

PM016 – 28 March 2024

Update on PINNs

Application to Urban Wind Field Dispersion Studies

Content

- 1) La Defense – POD Training Results
- 2) Treatment of POD
- 3) Why POD is not perfect & how to correct it
- 4) La Defense – Sampled Data Validation Results
- 5) La Defense – Full Dataset Validation Results

LA DEFENSE

Some Parameters

Infinite epochs - Simple Moving Average stopping condition

128 Neurons for the PINN unless otherwise specified (50949 parameters in total)

We have the data for 13 angles, [0, 15, 30, 45, 60, 75, 90, 105, 120, 135, 150, 165, 180] in degrees

We concatenate the data for angles = [0, 15, 30, 45, 60, 75, 90, 105, 120, 150, 165, 180] and then take 99% of the dataset with random seed = 42 for training and 1% for testing

By using 99% of the whole dataset we hope to make the NN learn about wind angle such that the parameters become functions of the wind angle

Then using the trained neural network we predict the data for angle = 135

For this run, we will only have input parameters to be [X, Y, Z, cos(\theta), sin(\theta)] and the output parameters will be [U, V, W] (for the POD dataset we have [Pressure, U, V, W, TurbVisc])

Total Number of Data Points → 1.21954E7 points per wind angle * (5 inputs + 3 outputs) * (12 training wind angles) ~ 1.17E9 (~1.46E9 if we include Pressure and TurbVisc)

Progress so far - Data Loss Only
Standard Normal Scalar – ELU Activation
(Adam Optimizer)

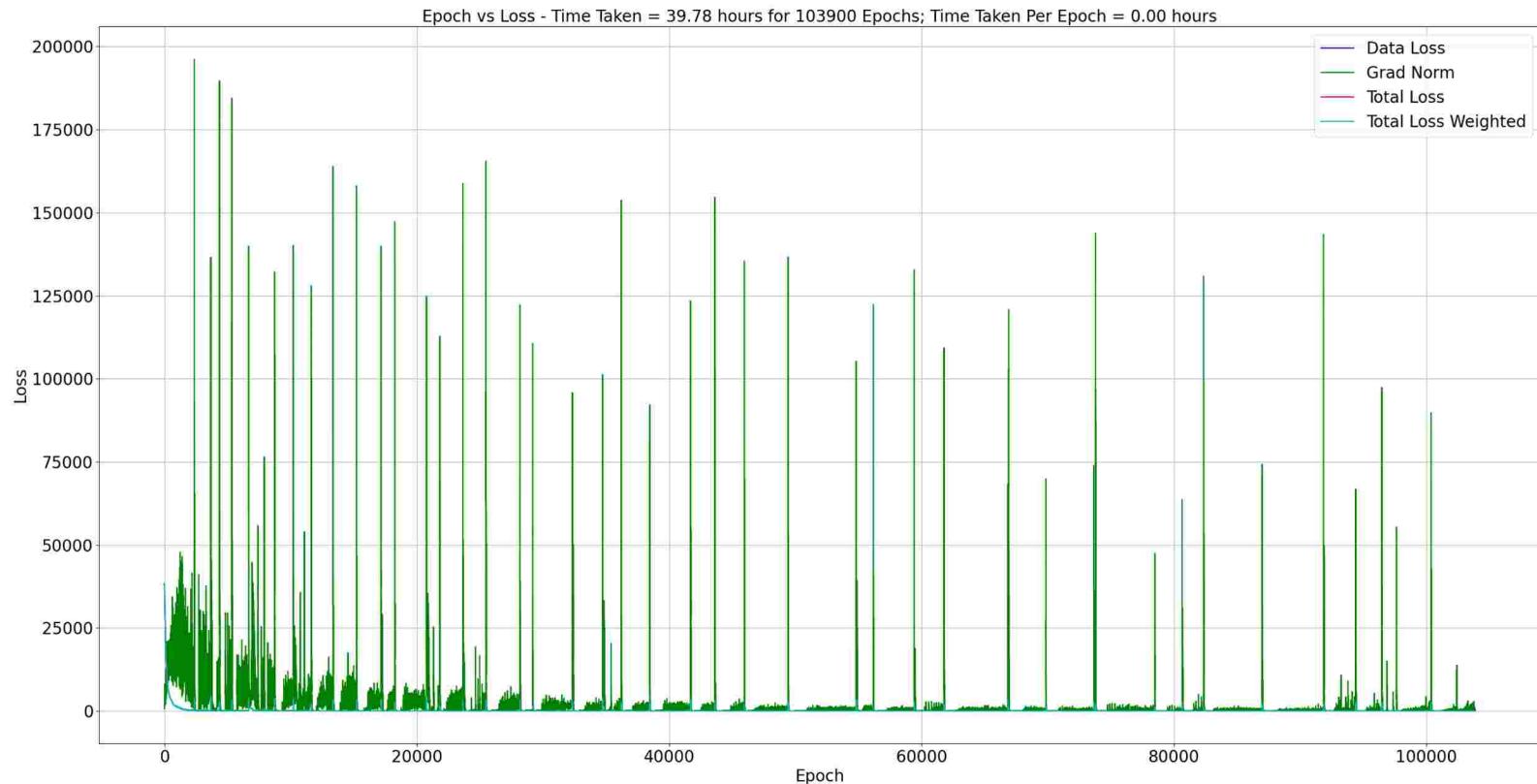
POD Dataset, GPU Laptop
103900 Epochs

Scripts v5 – TESTING

Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

103900 Epochs, GPU Laptop

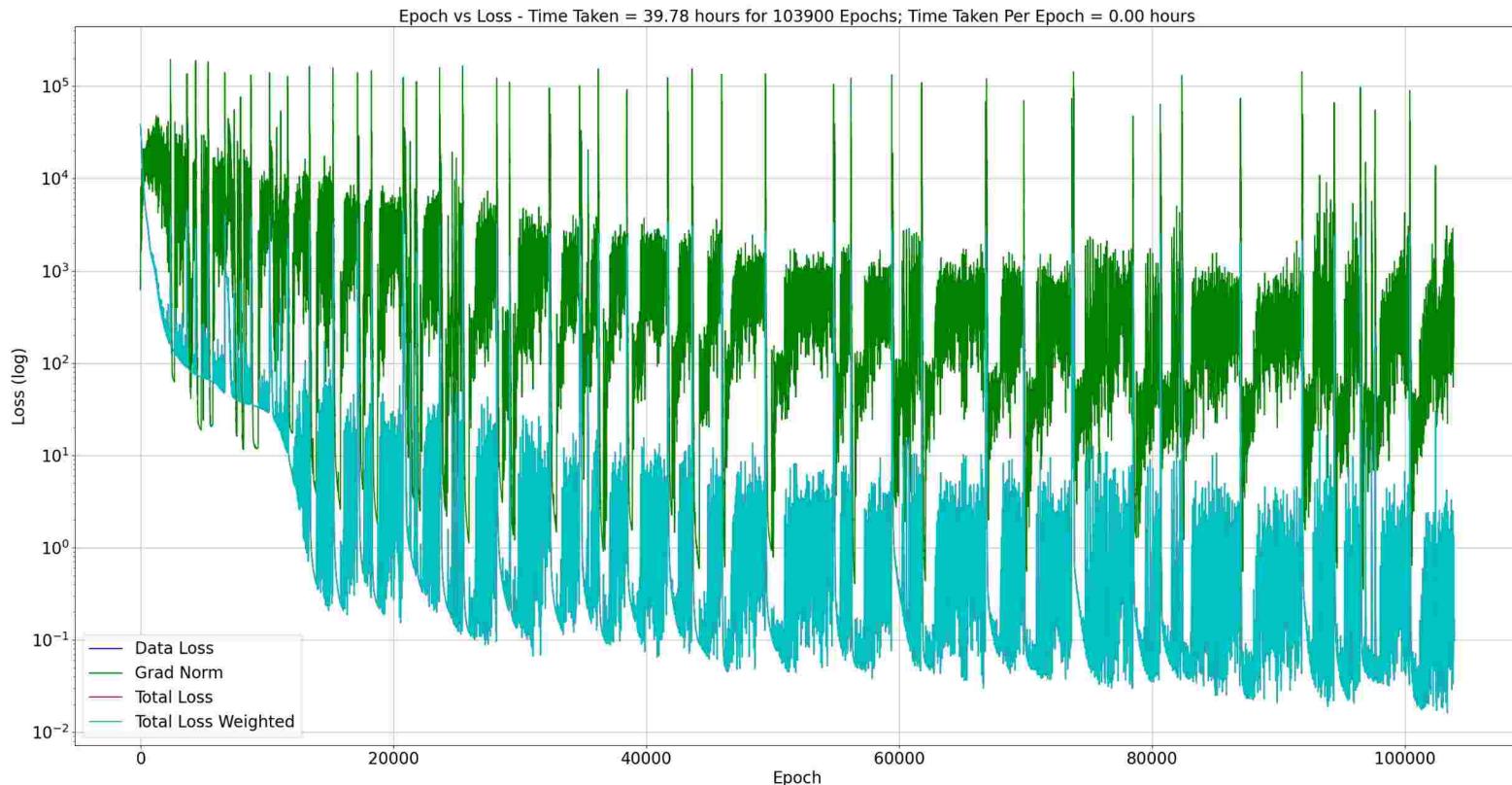
Data Loss w Grad Norm Plot



Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

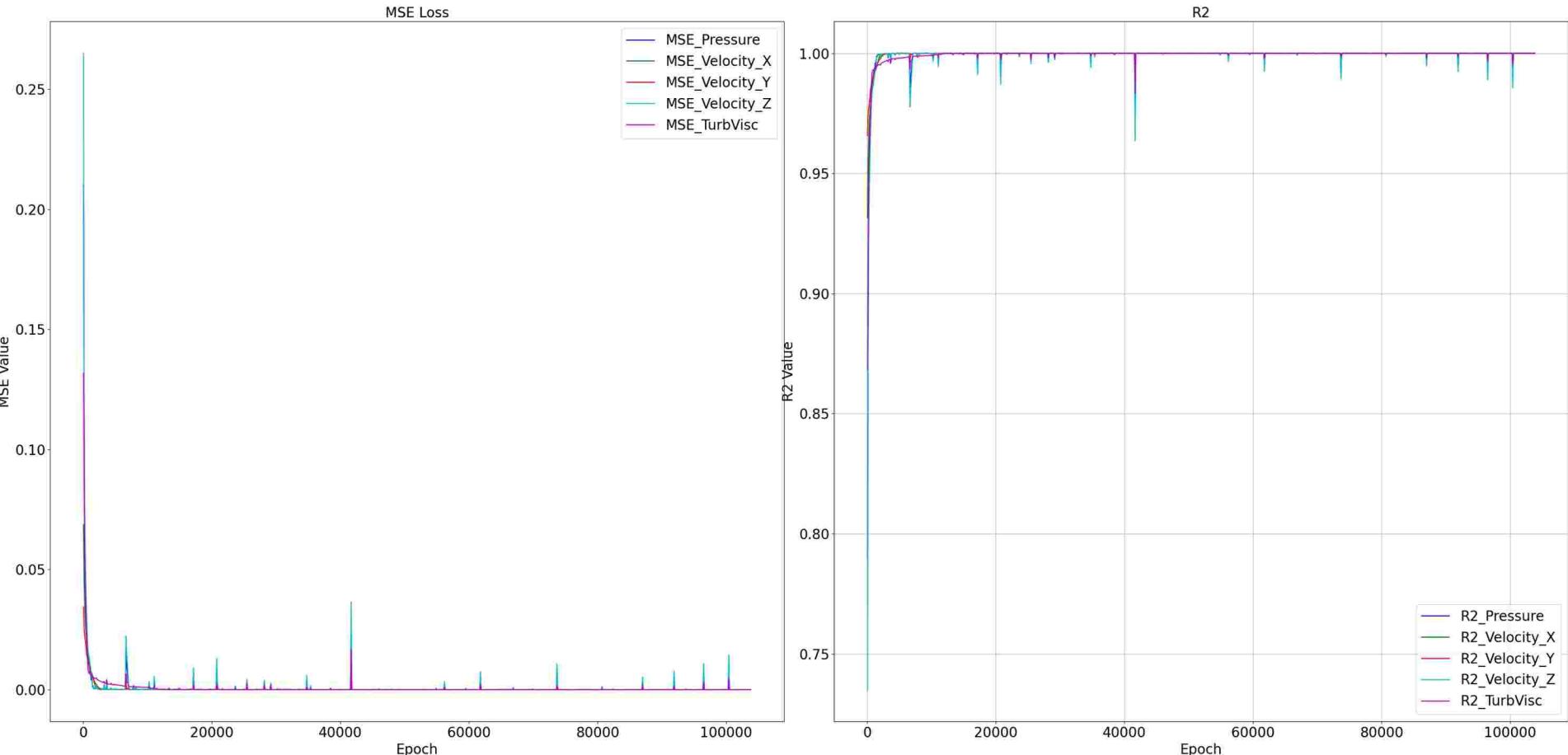
103900 Epochs, GPU Laptop

Data Loss w Grad Norm Plot



Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
103900 Epochs, GPU Laptop
Training MSE & R2 Results

Time Taken = 39.78 hours for 103900 Epochs; Time Taken Per Epoch = 0.00 hours

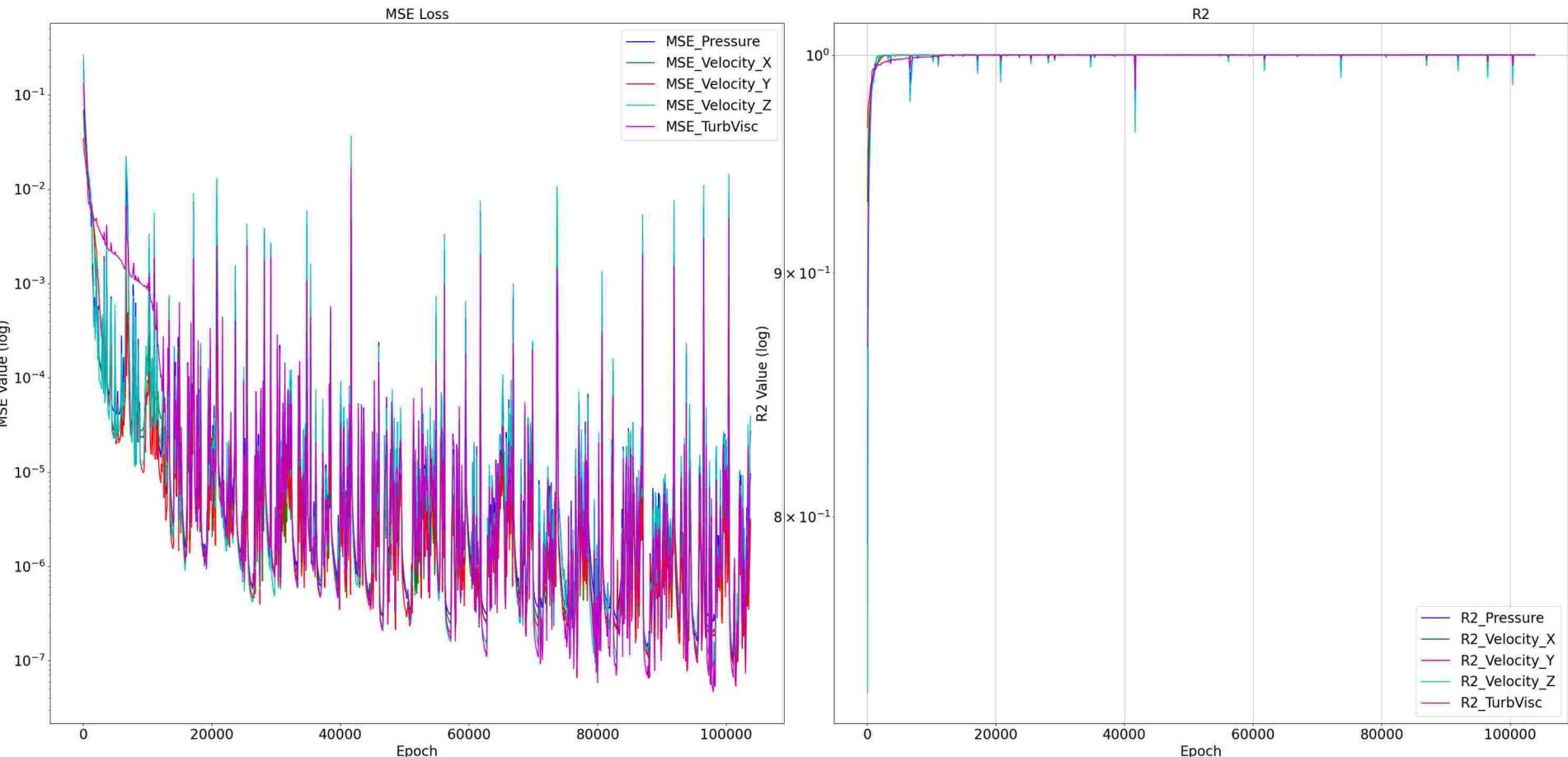


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

103900 Epochs, GPU Laptop

Training MSE & R2 Results

Time Taken = 39.78 hours for 103900 Epochs; Time Taken Per Epoch = 0.00 hours

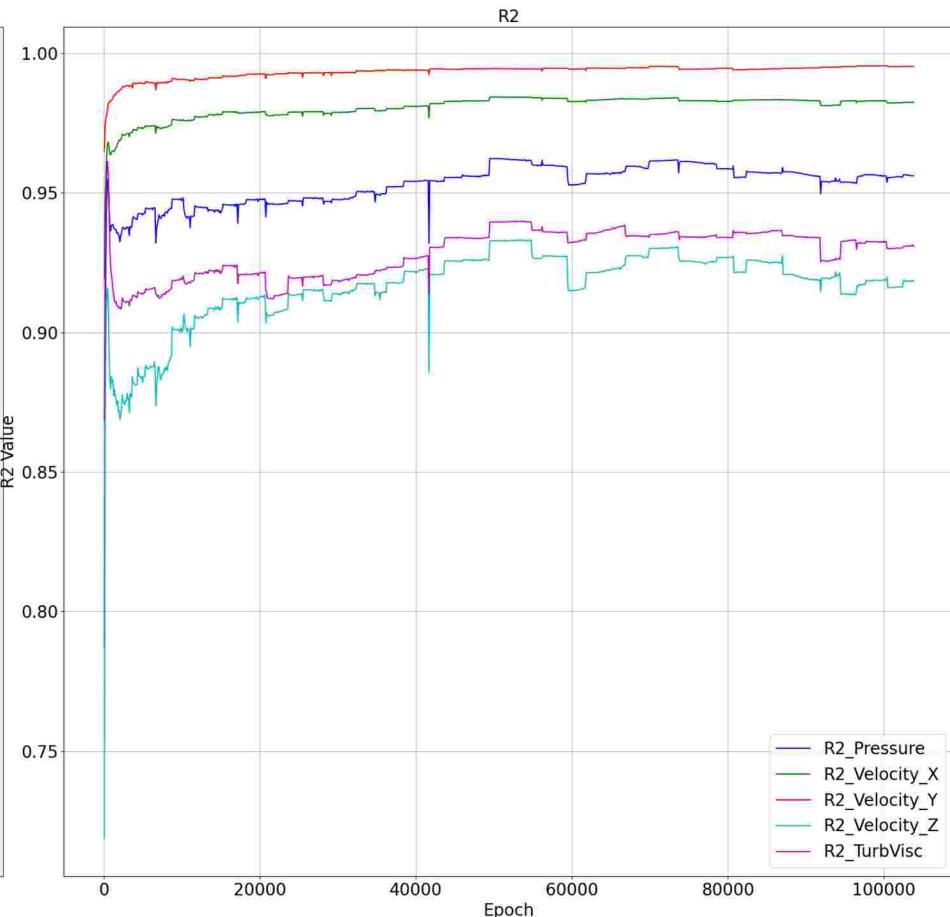
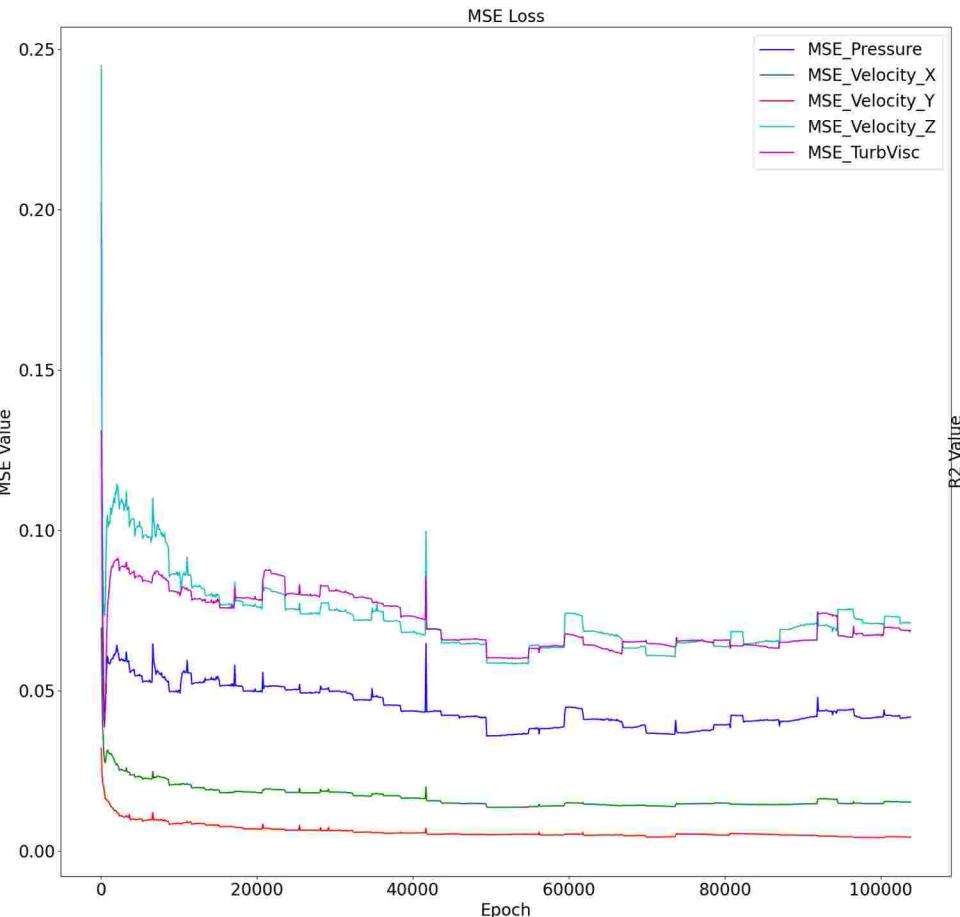


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

103900 Epochs, GPU Laptop

Skipped MSE & R2 Results

Time Taken = 39.78 hours for 103900 Epochs; Time Taken Per Epoch = 0.00 hours



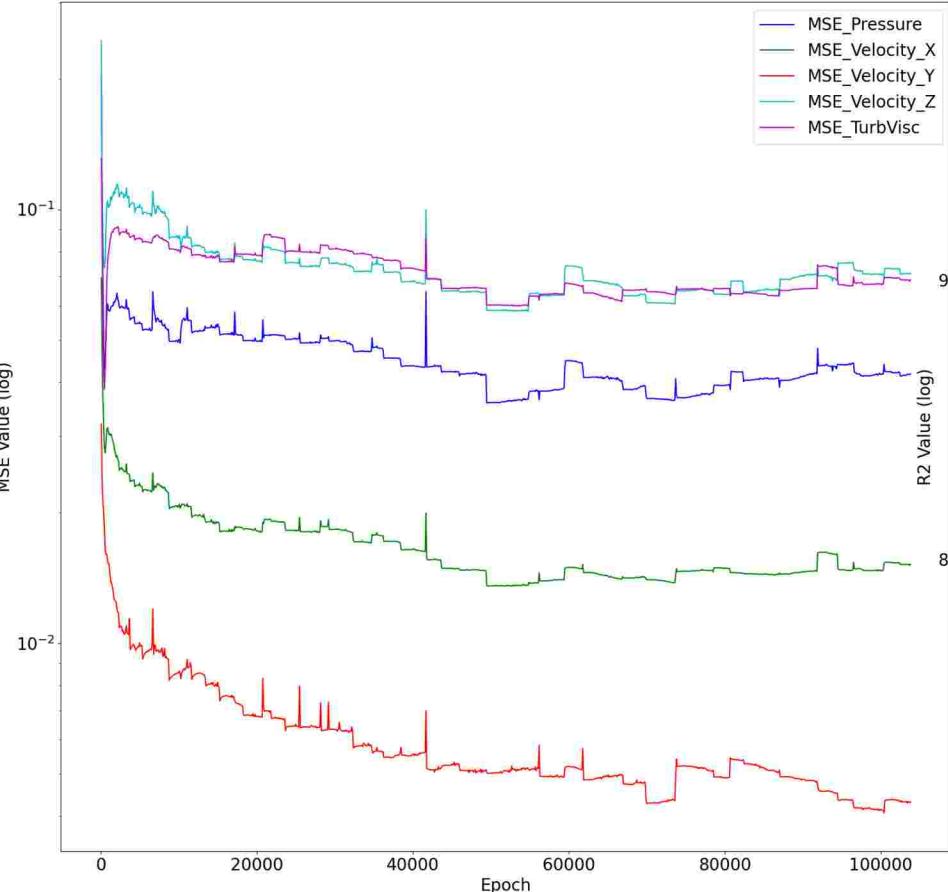
Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

103900 Epochs, GPU Laptop

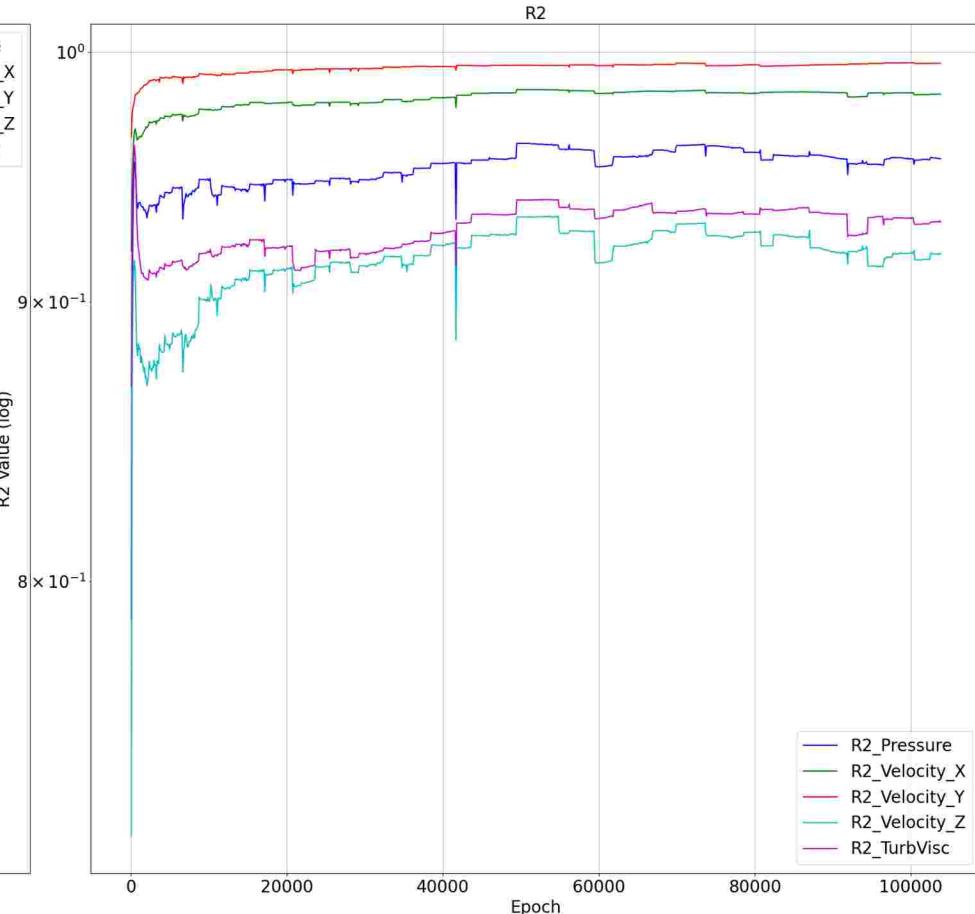
Skipped MSE & R2 Results

Time Taken = 39.78 hours for 103900 Epochs; Time Taken Per Epoch = 0.00 hours

MSE Loss

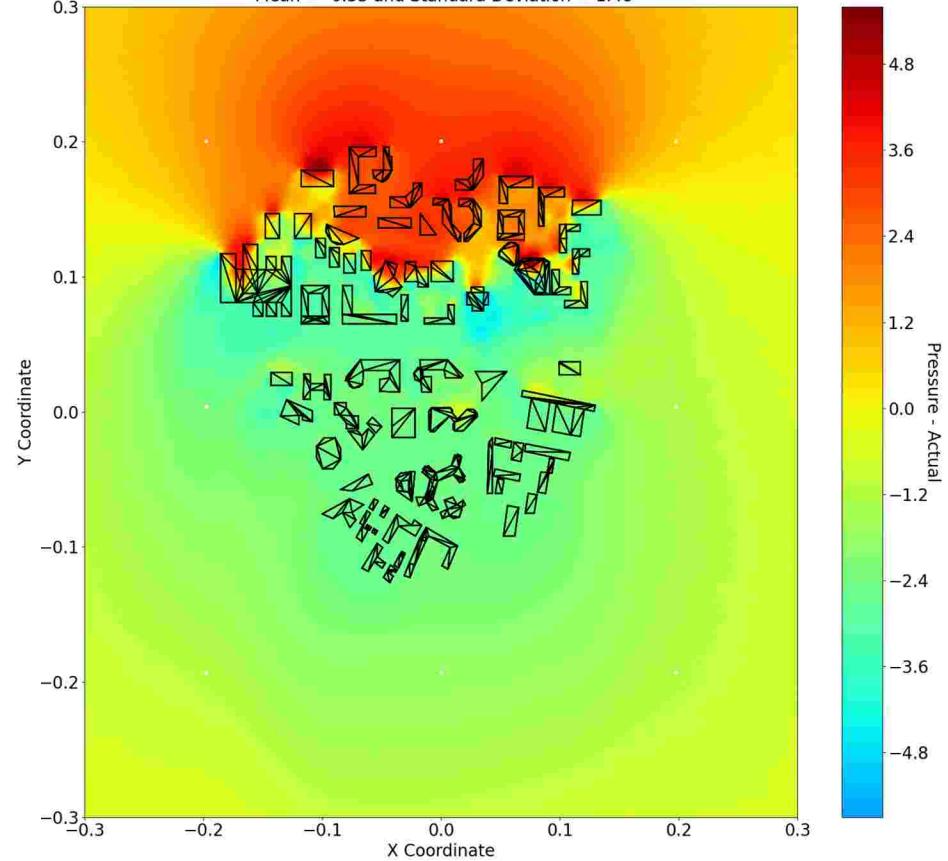


R2

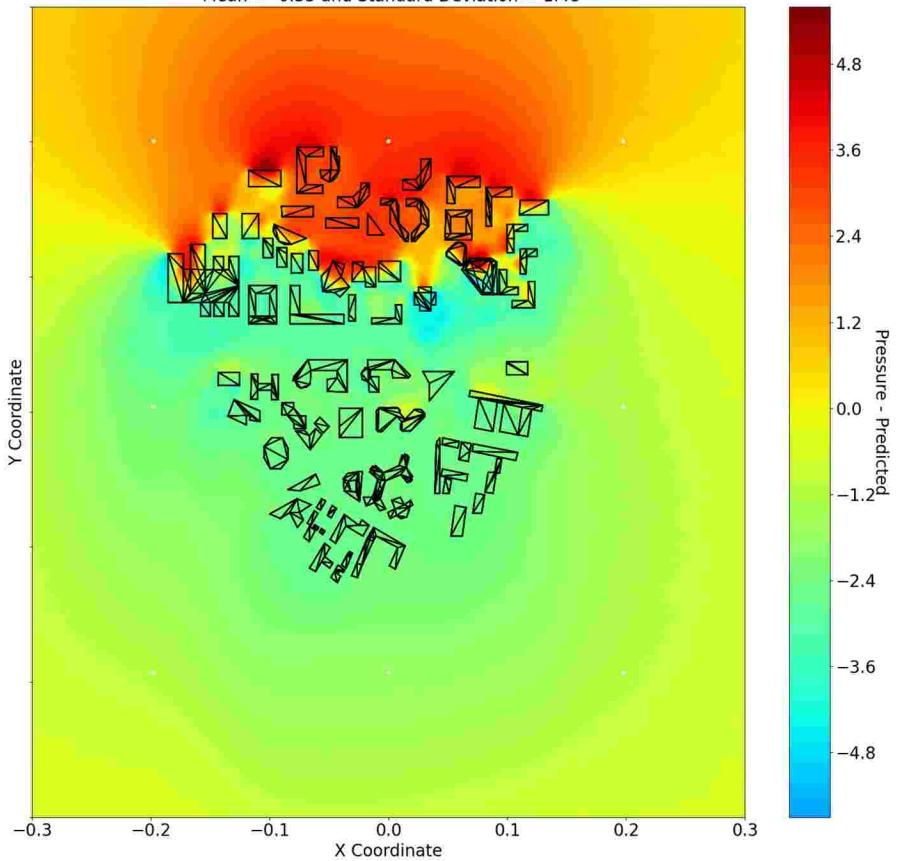


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Pressure in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = -0.33 and Standard Deviation = 1.48

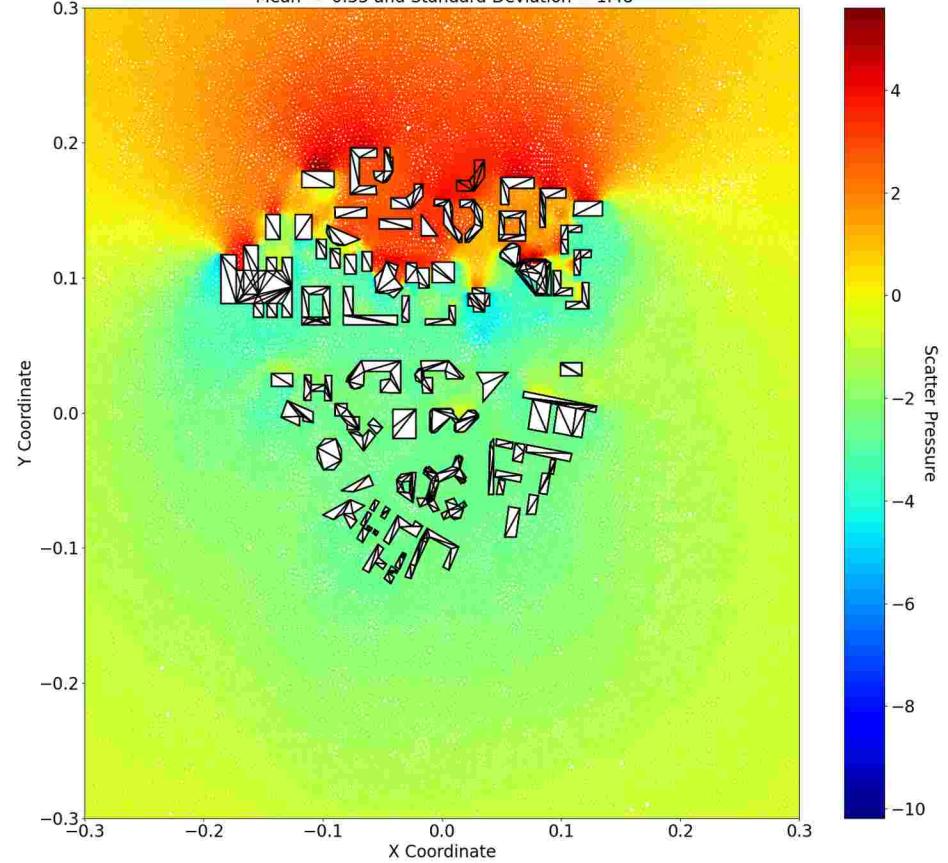


Predicted Pressure in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
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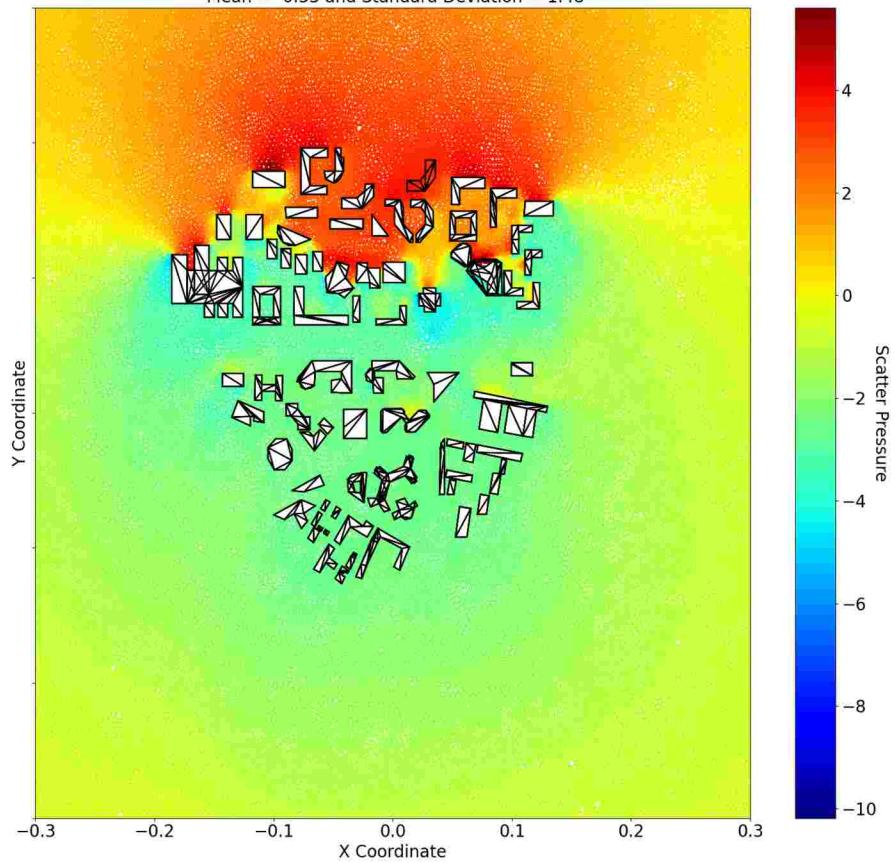


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

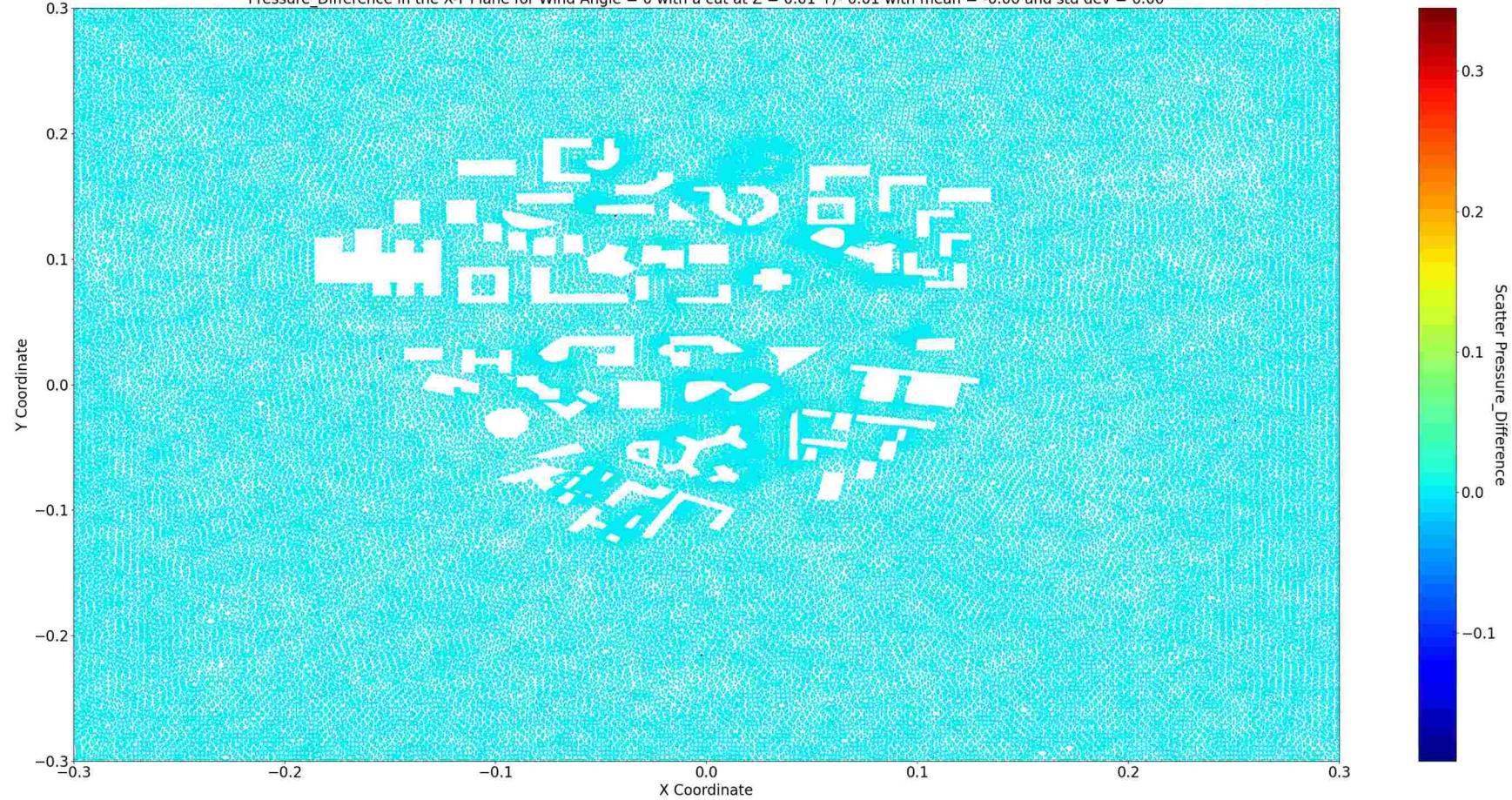
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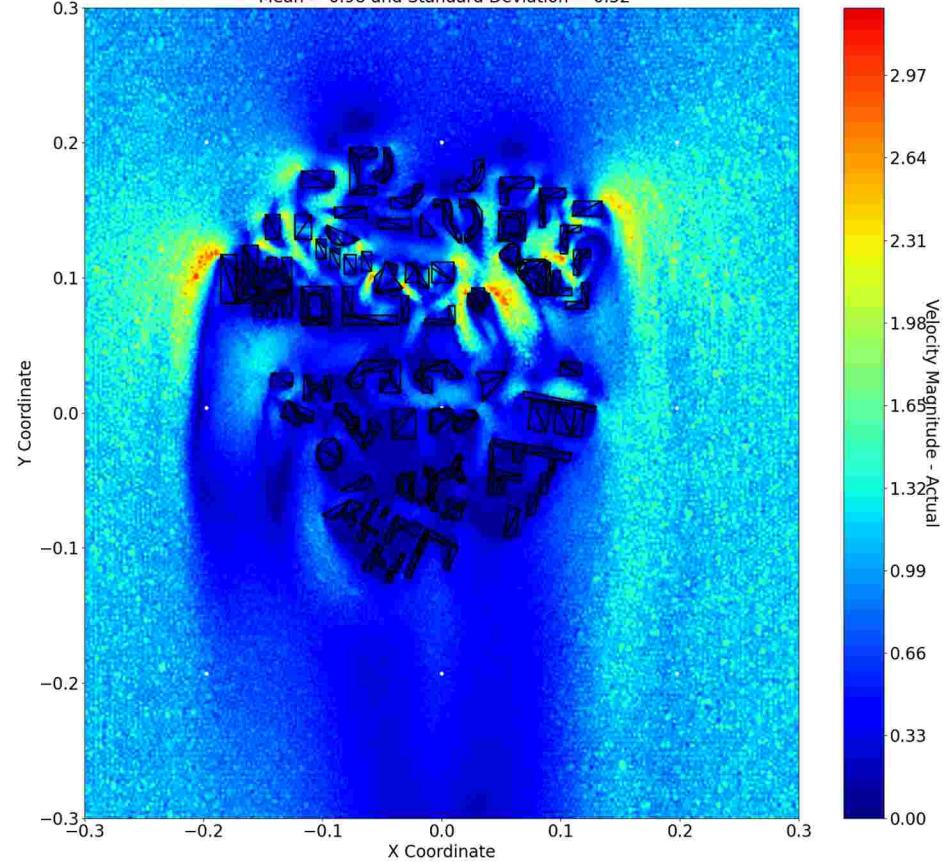


Pressure_Difference in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01 with mean = -0.00 and std dev = 0.00

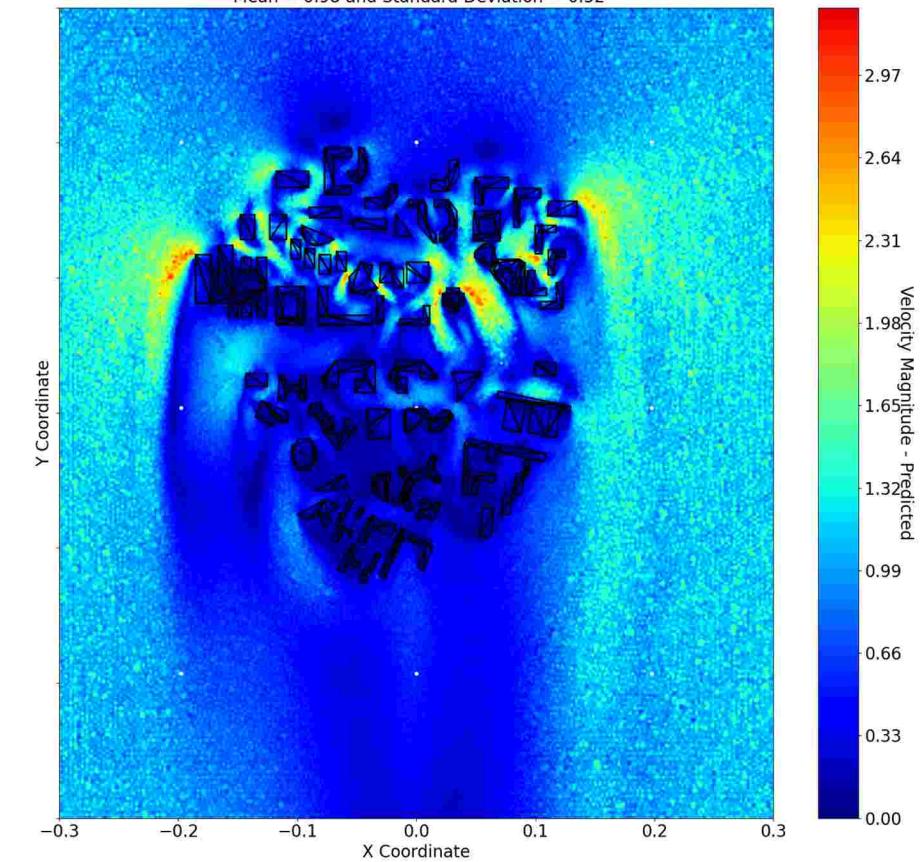


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.98 and Standard Deviation = 0.52

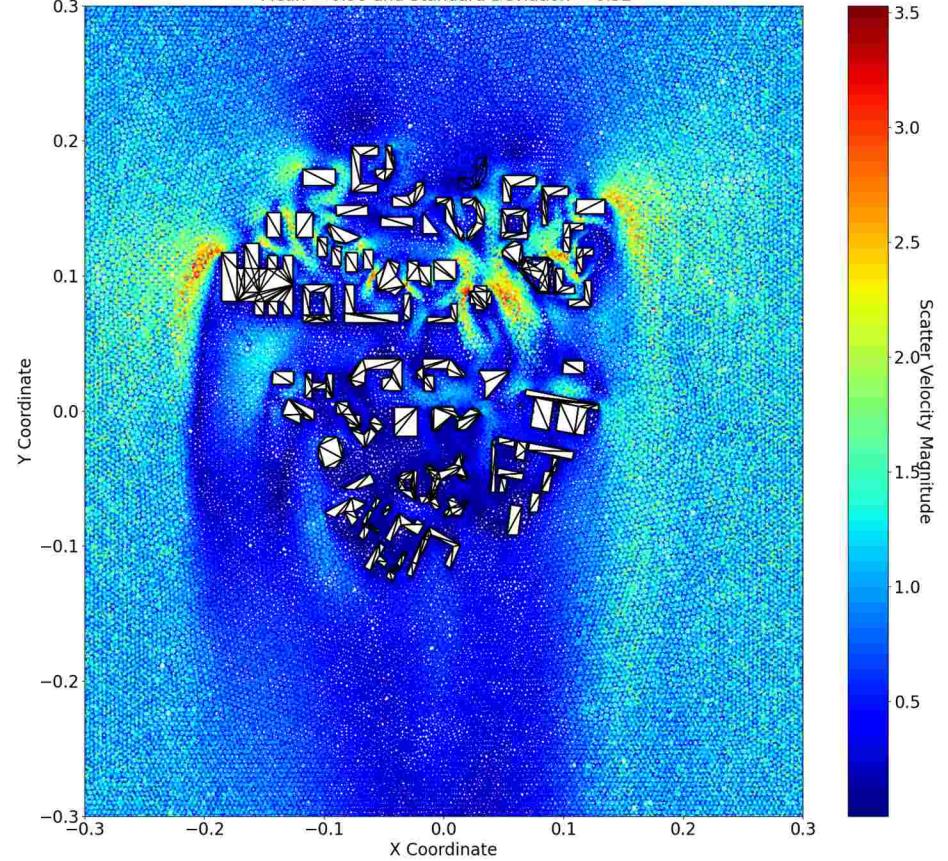


Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.98 and Standard Deviation = 0.52

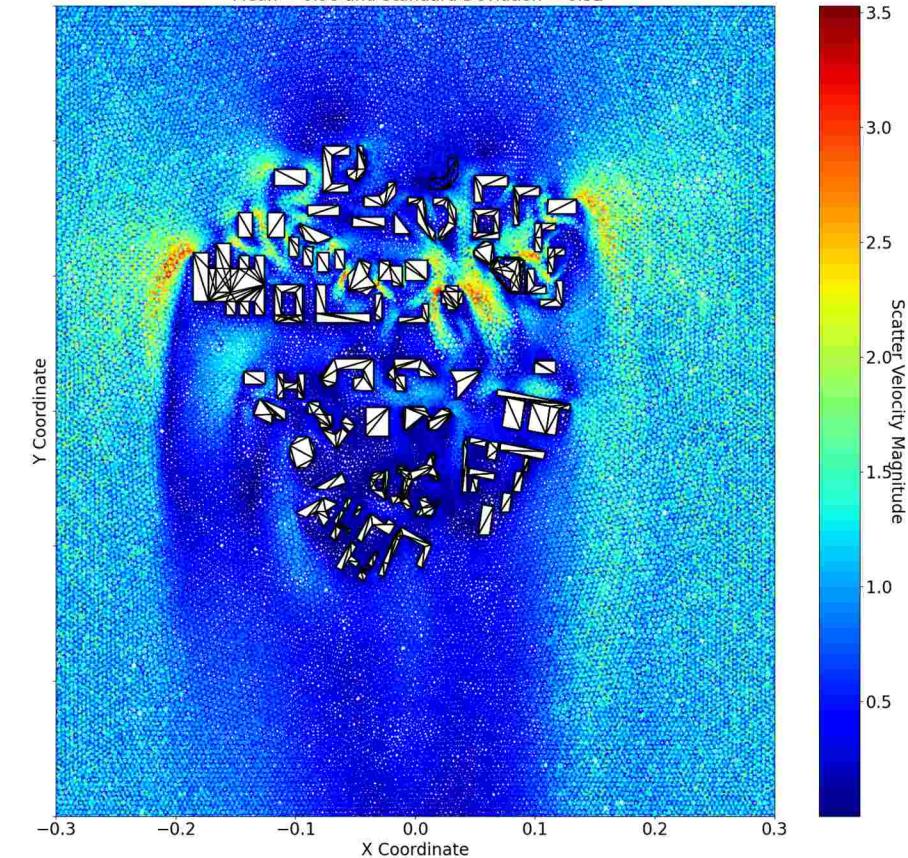


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

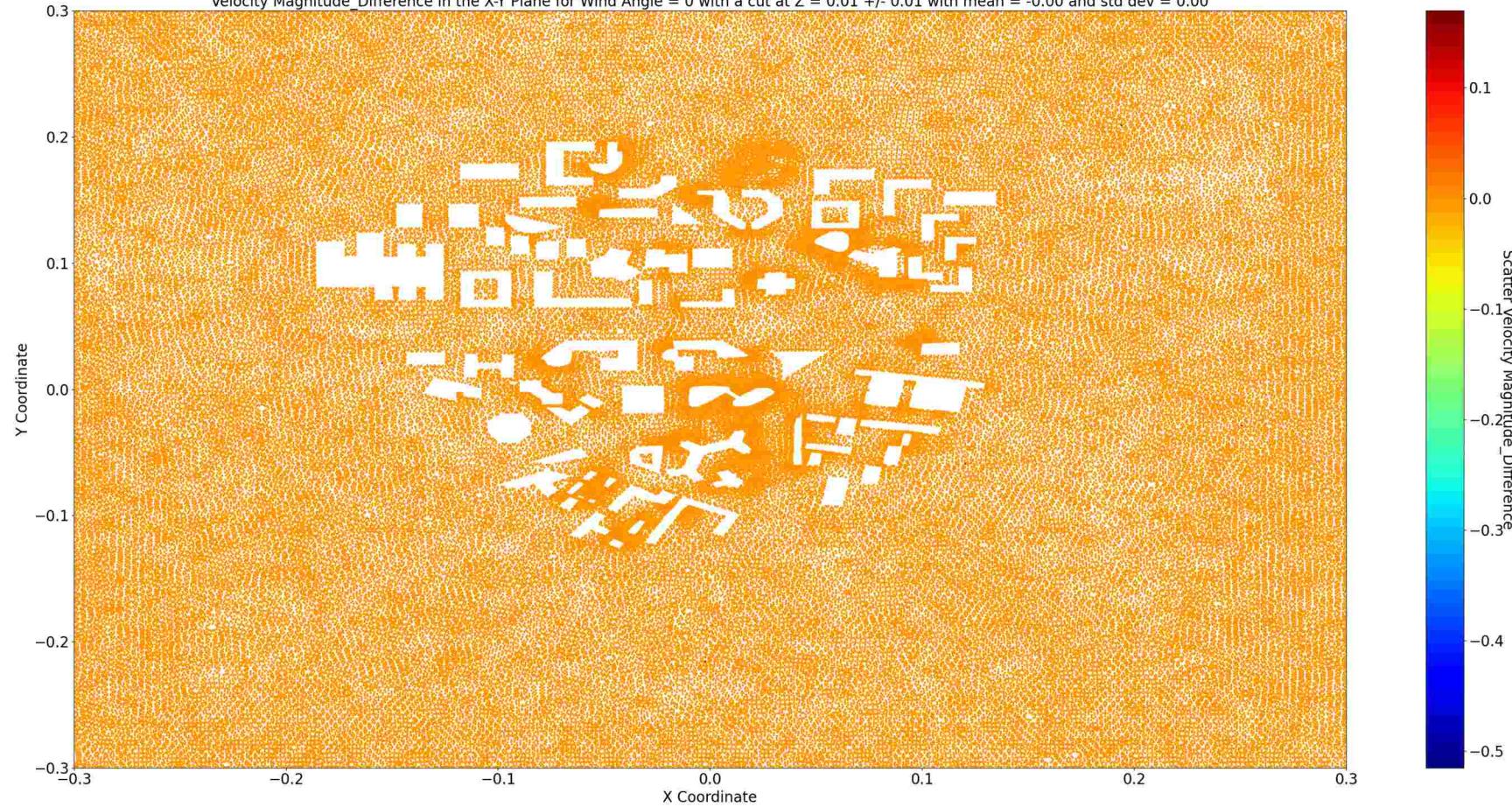
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Mean = 0.98 and Standard Deviation = 0.52

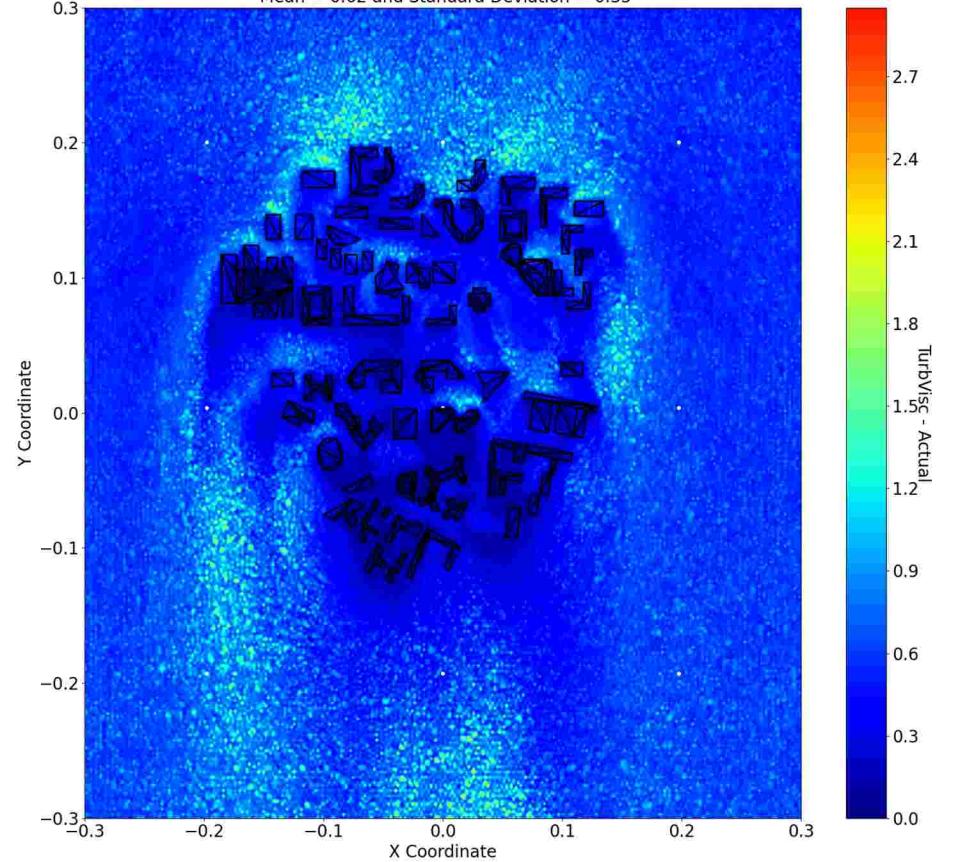


Velocity Magnitude Difference in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01 with mean = -0.00 and std dev = 0.00

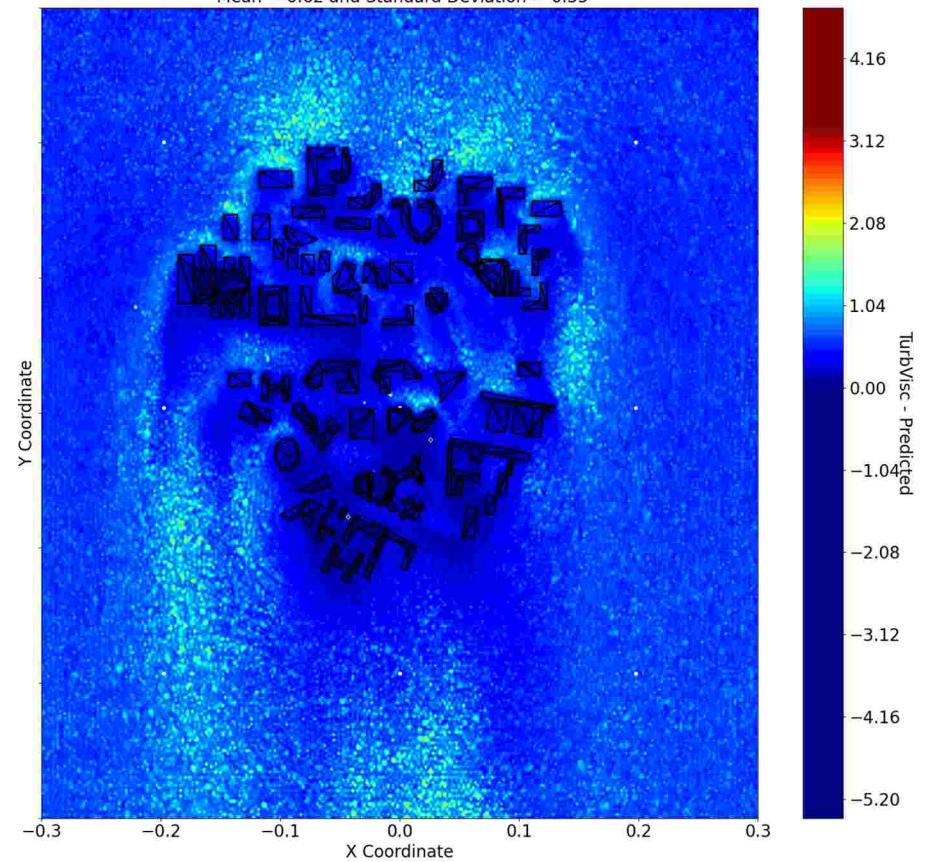


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual TurbVisc in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.62 and Standard Deviation = 0.35

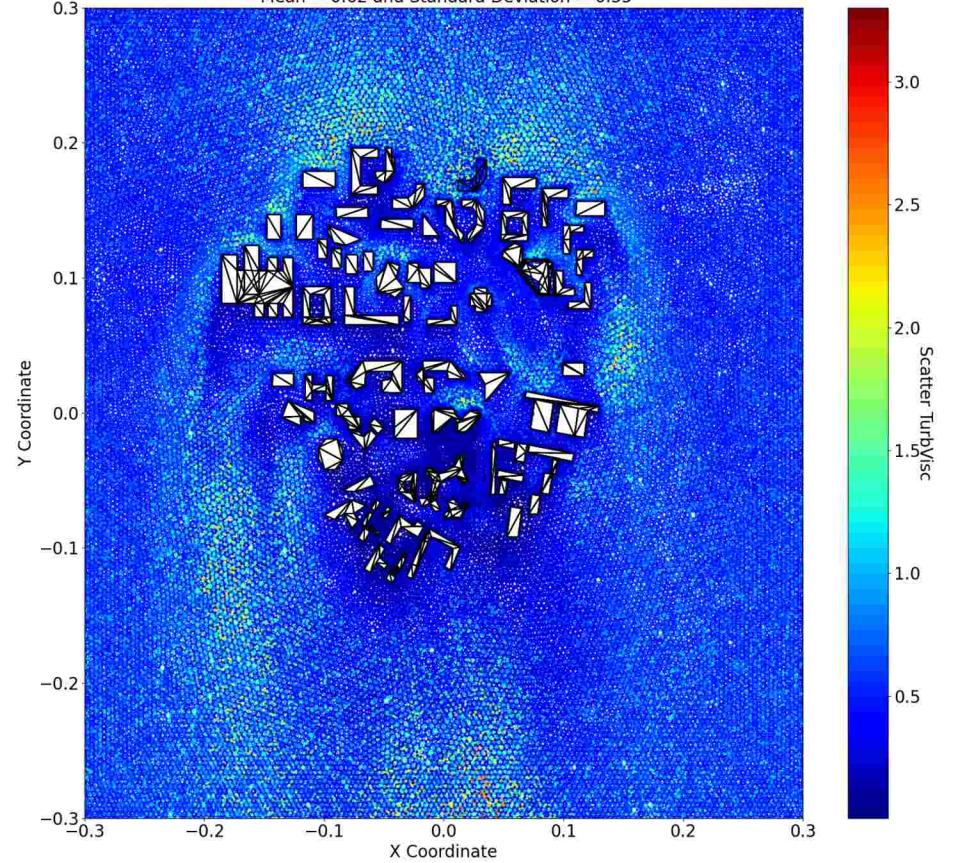


Predicted TurbVisc in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.62 and Standard Deviation = 0.35

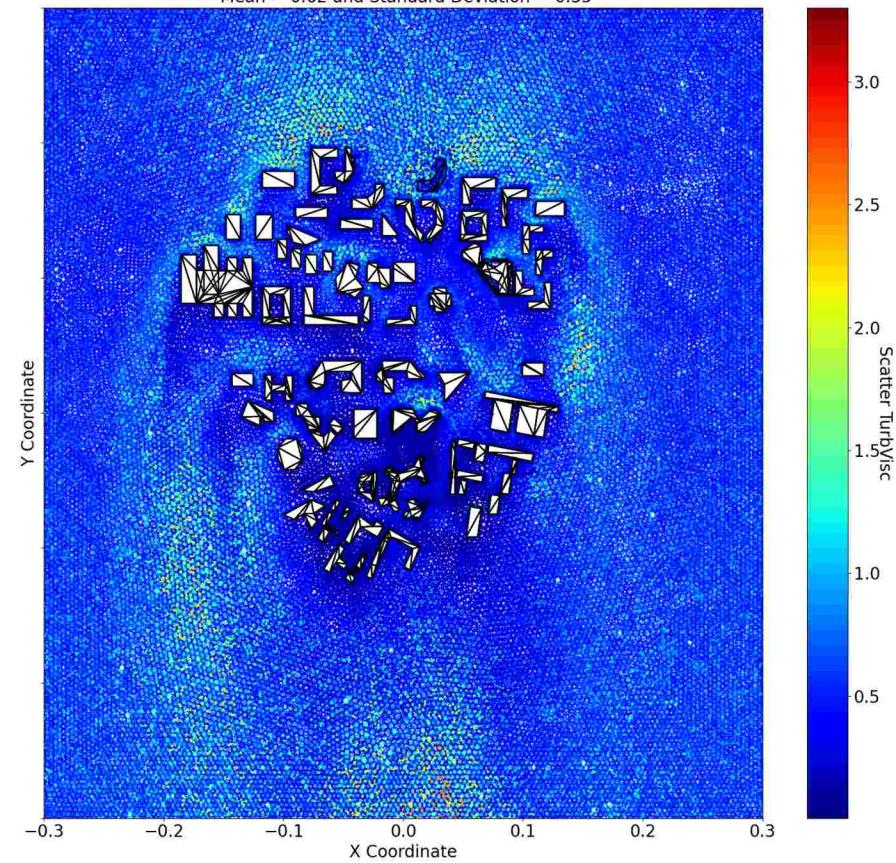


Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

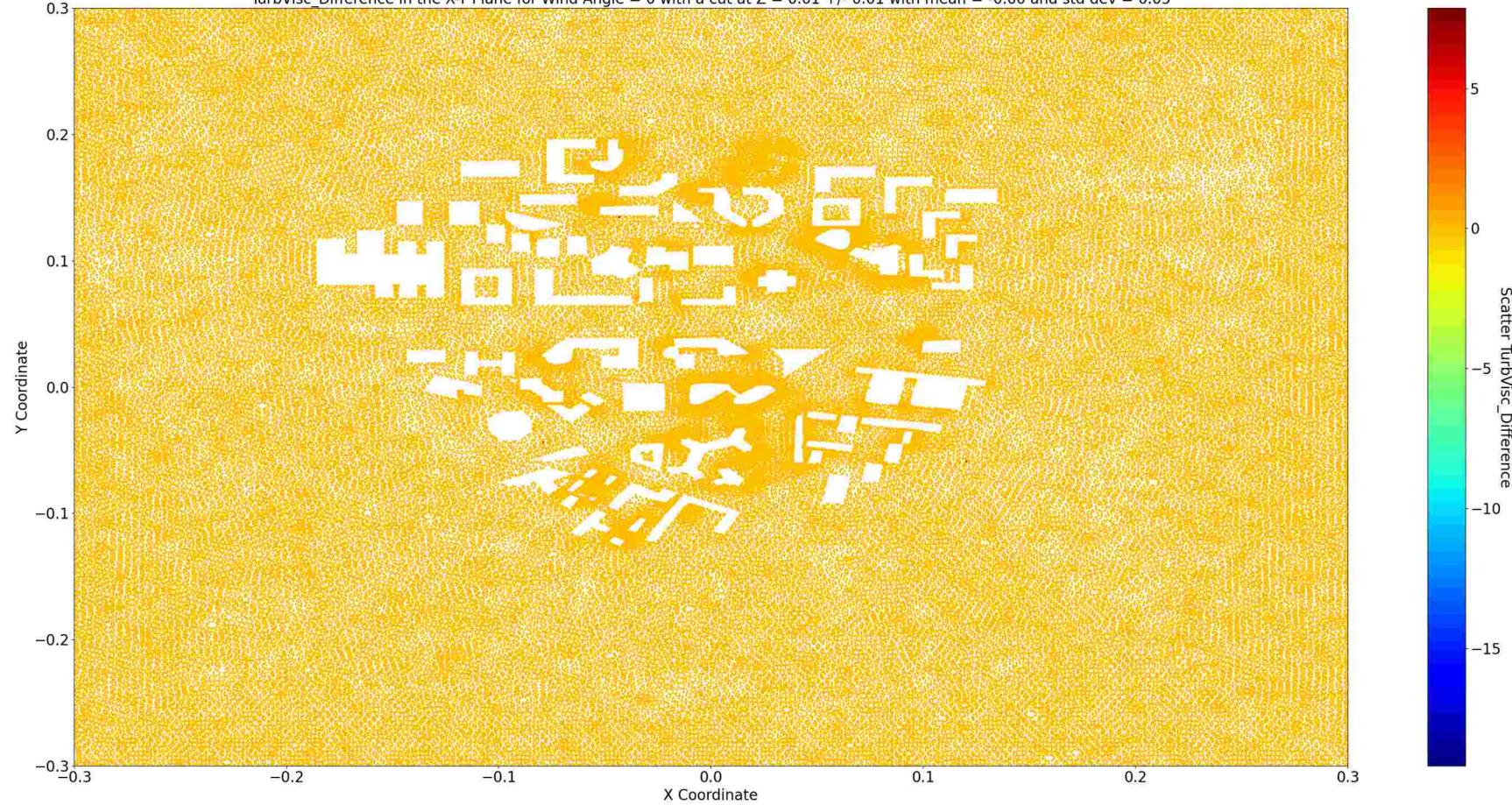
Actual TurbVisc in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.62 and Standard Deviation = 0.35



Predicted TurbVisc in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01
Mean = 0.62 and Standard Deviation = 0.35



TurbVisc_Difference in the X-Y Plane for Wind Angle = 0 with a cut at Z = 0.01 +/- 0.01 with mean = -0.00 and std dev = 0.05



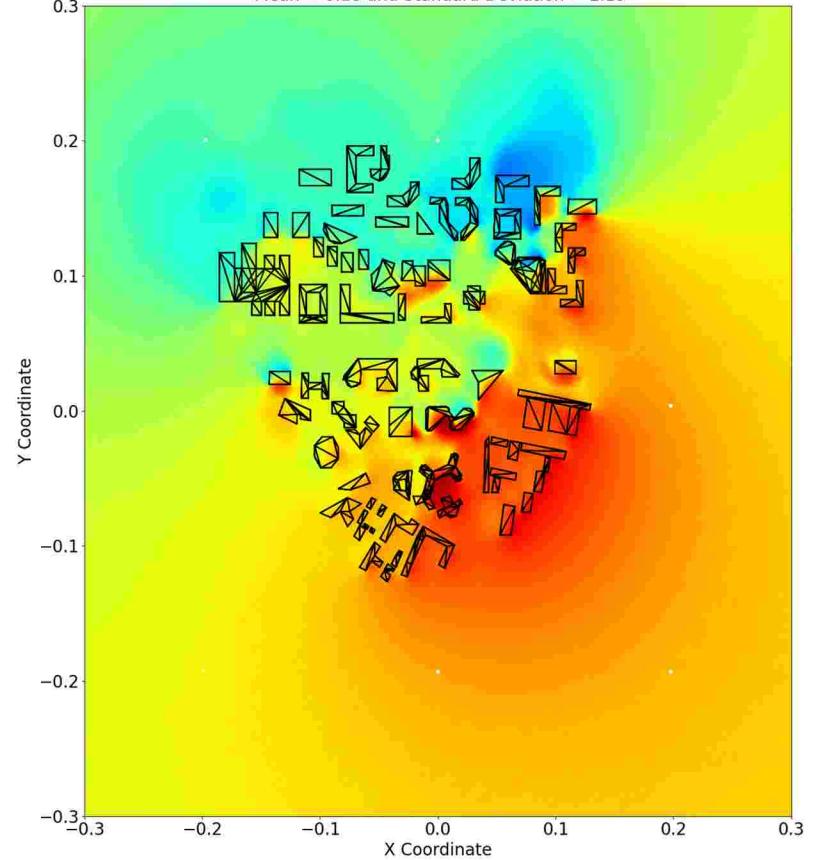
Progress so far - Data Loss Only
Standard Normal Scalar – ELU Activation
(Adam Optimizer)

POD Dataset, GPU Laptop
103900 Epochs

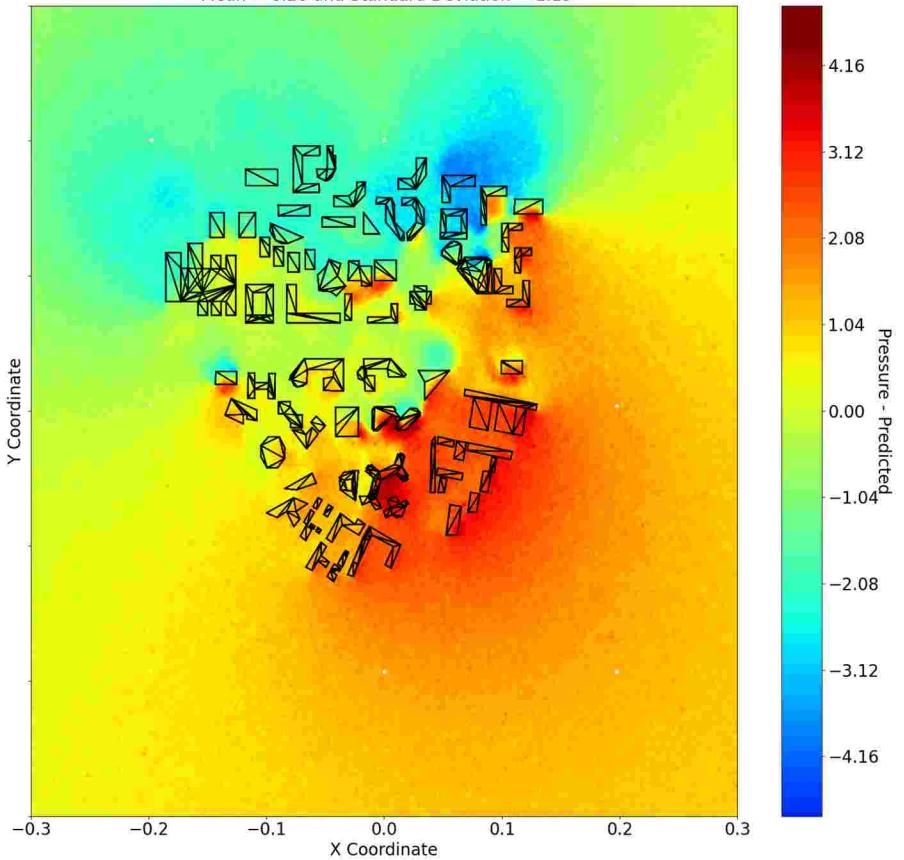
Scripts v5 – VALIDATION (135)

Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Pressure in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.18 and Standard Deviation = 1.19

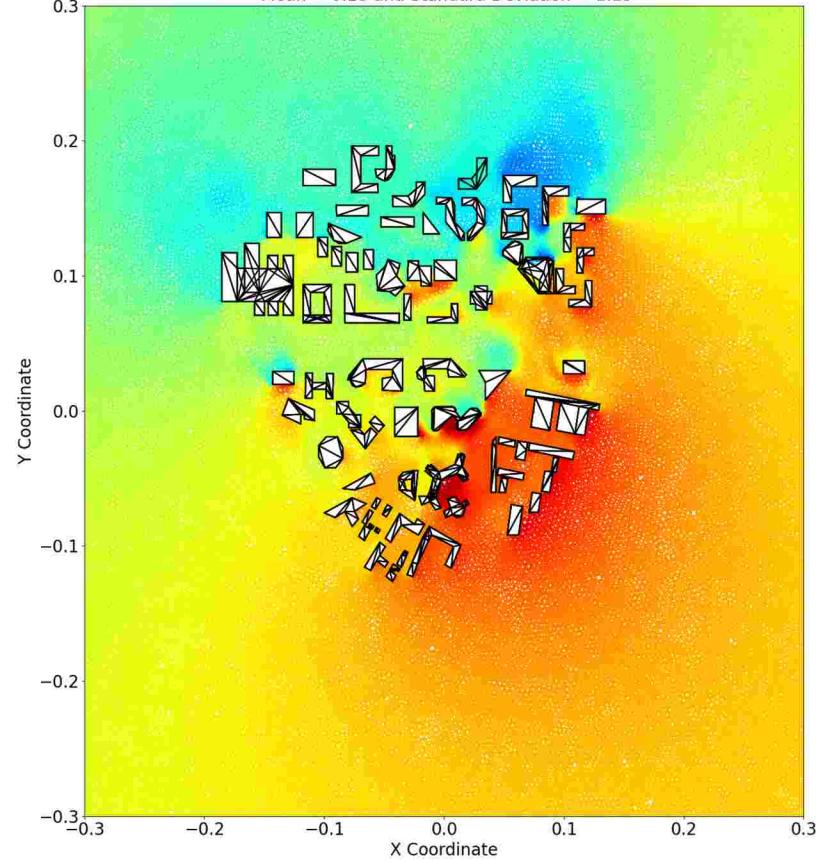


Predicted Pressure in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.20 and Standard Deviation = 1.19

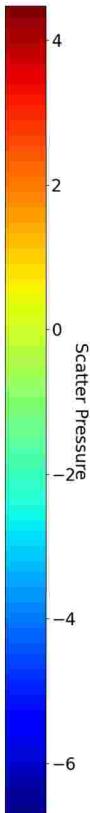
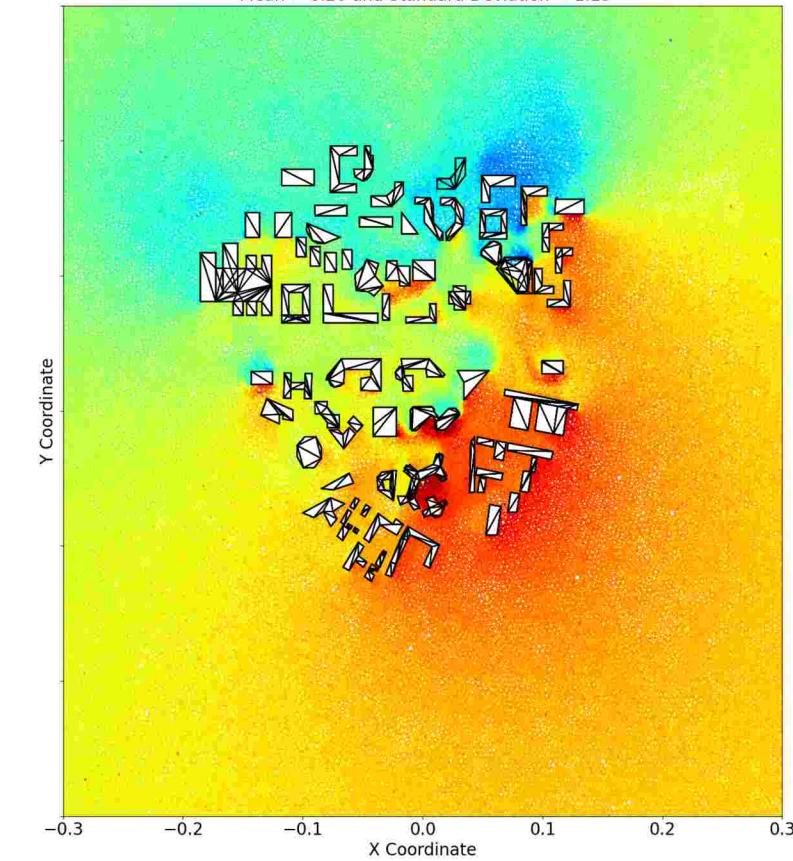


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

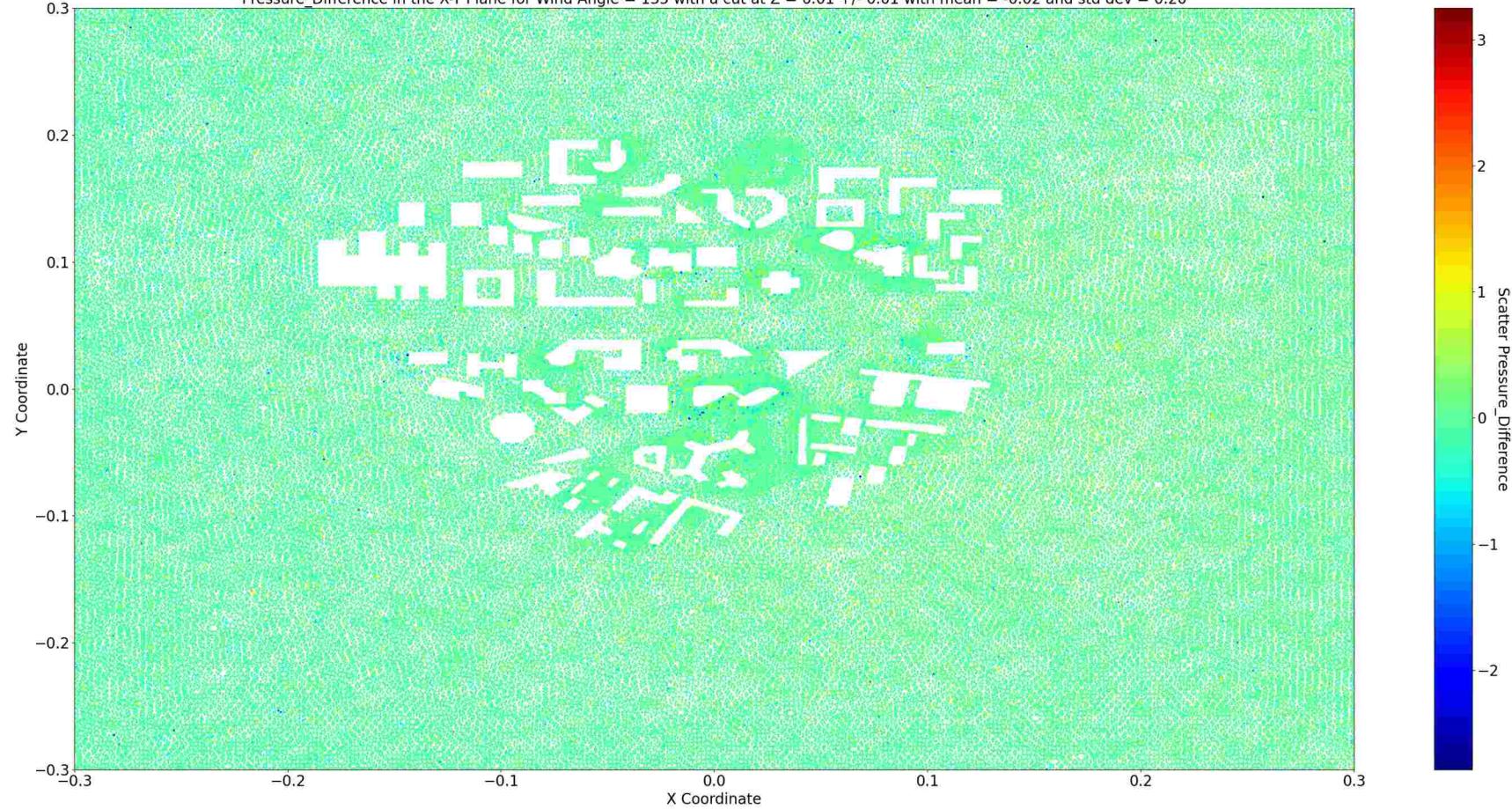
Actual Pressure in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.18 and Standard Deviation = 1.19



Predicted Pressure in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.20 and Standard Deviation = 1.19

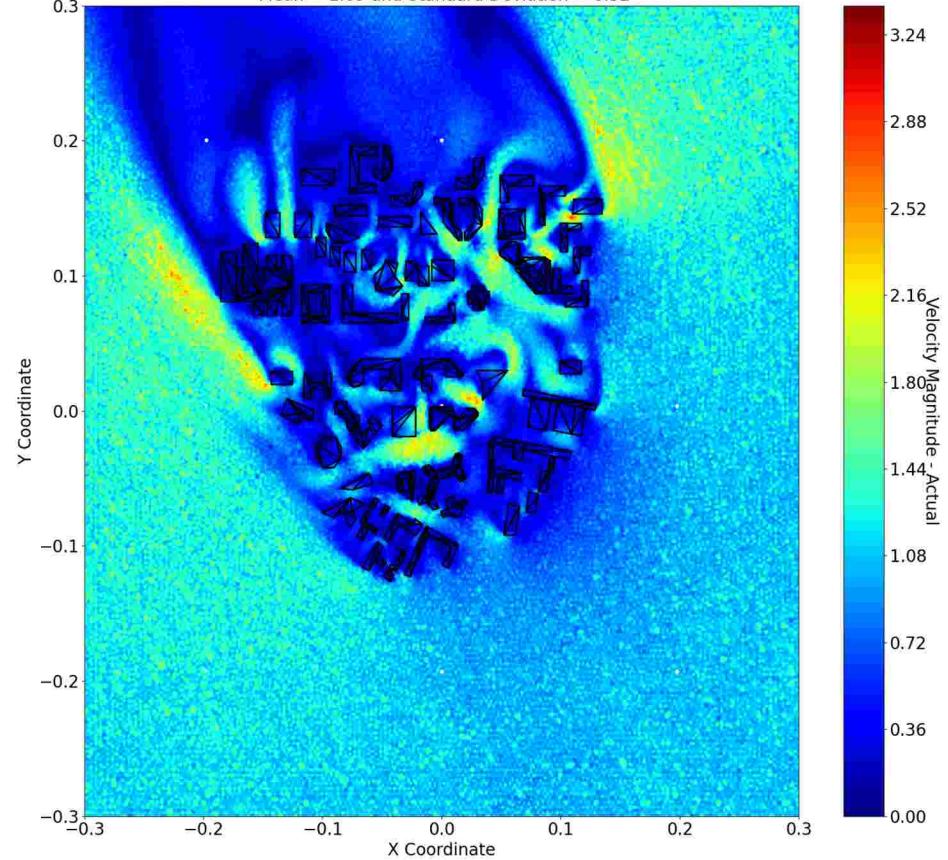


Pressure Difference in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01 with mean = -0.02 and std dev = 0.20

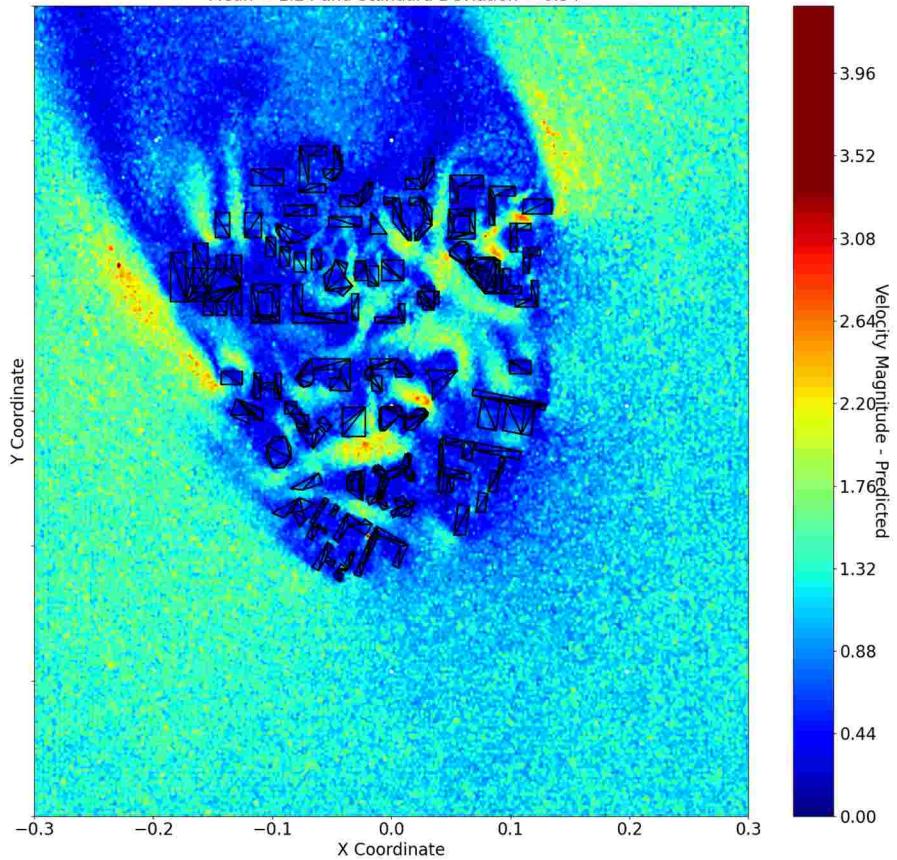


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.09 and Standard Deviation = 0.52

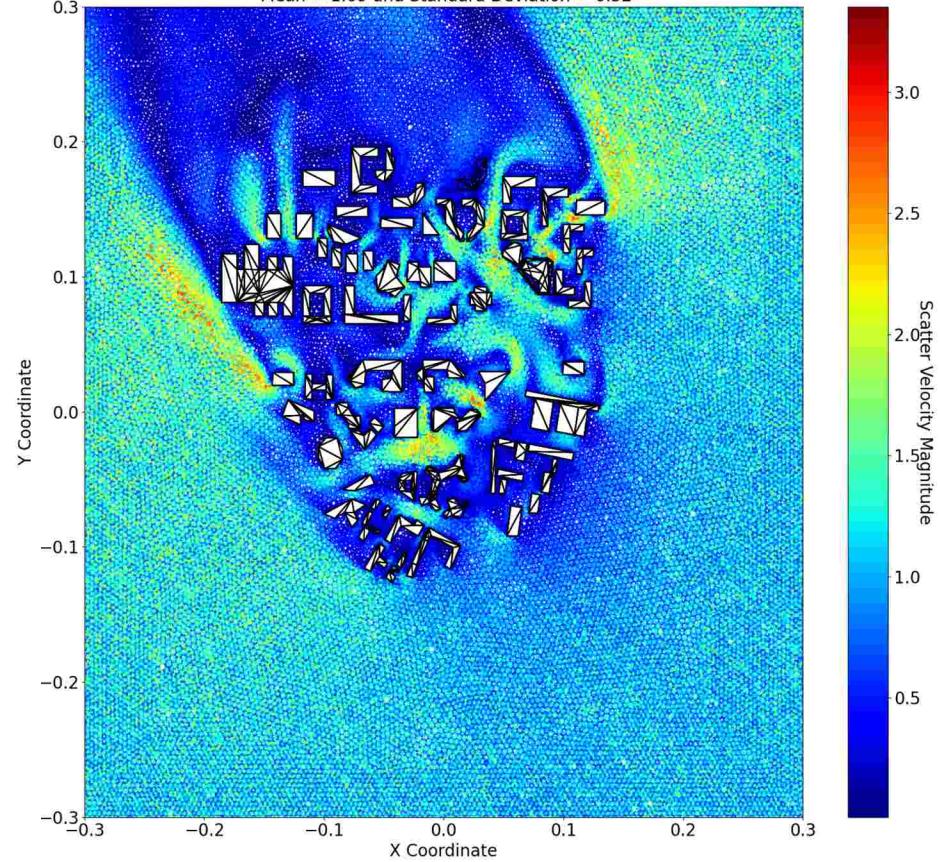


Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.24 and Standard Deviation = 0.54

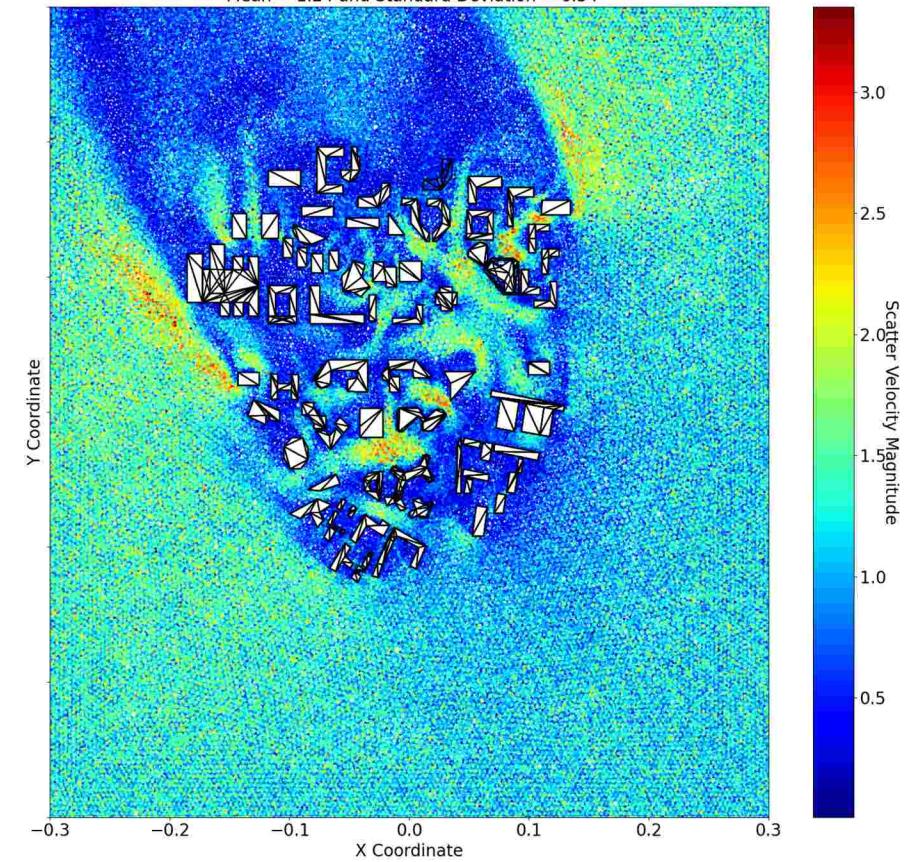


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

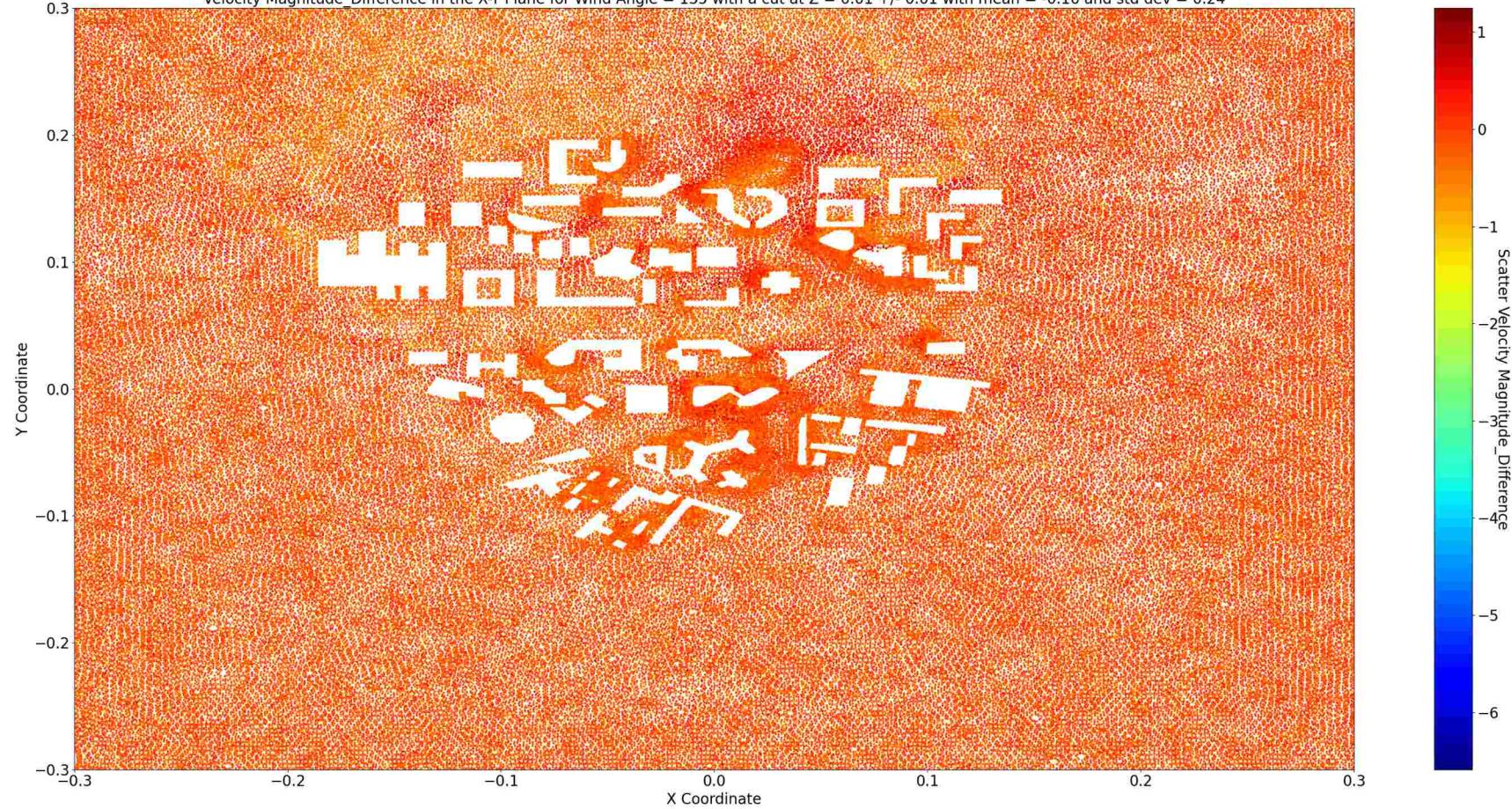
Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.09 and Standard Deviation = 0.52



Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.24 and Standard Deviation = 0.54

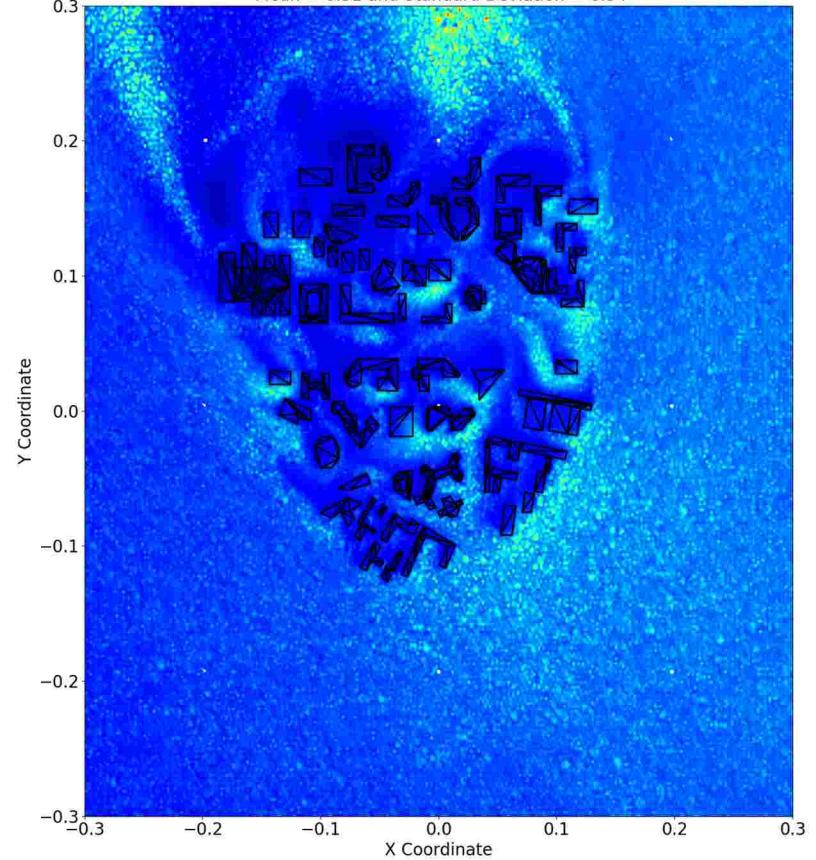


Velocity Magnitude Difference in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01 with mean = -0.16 and std dev = 0.24

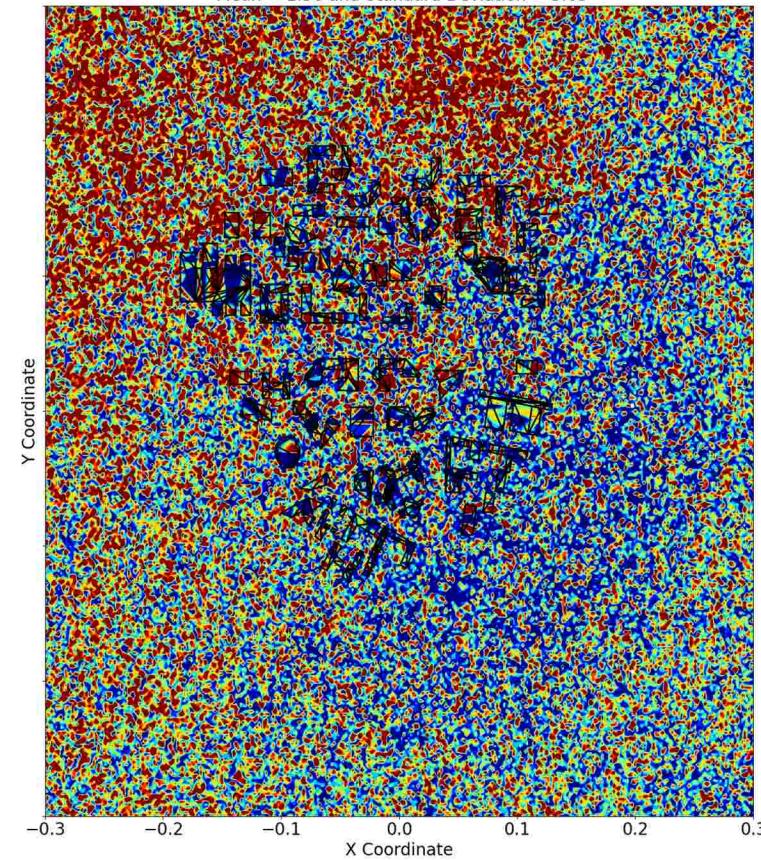


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual TurbVisc in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.51 and Standard Deviation = 0.34



Predicted TurbVisc in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.56 and Standard Deviation = 3.63

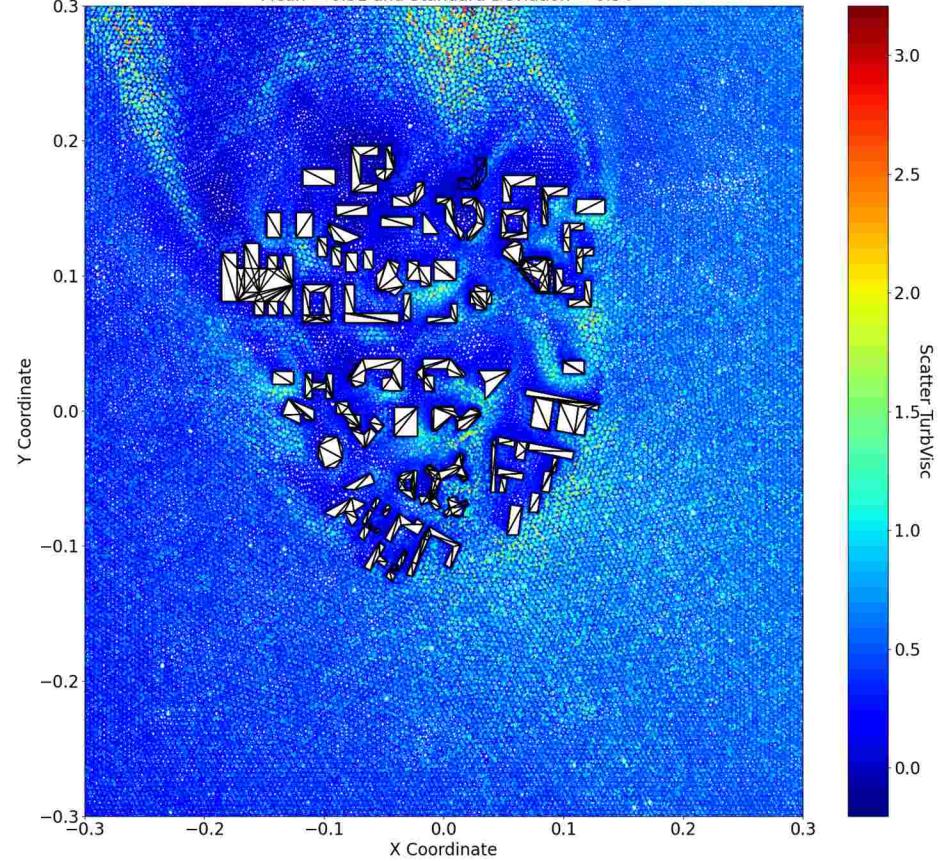


TurbVisc - Predicted

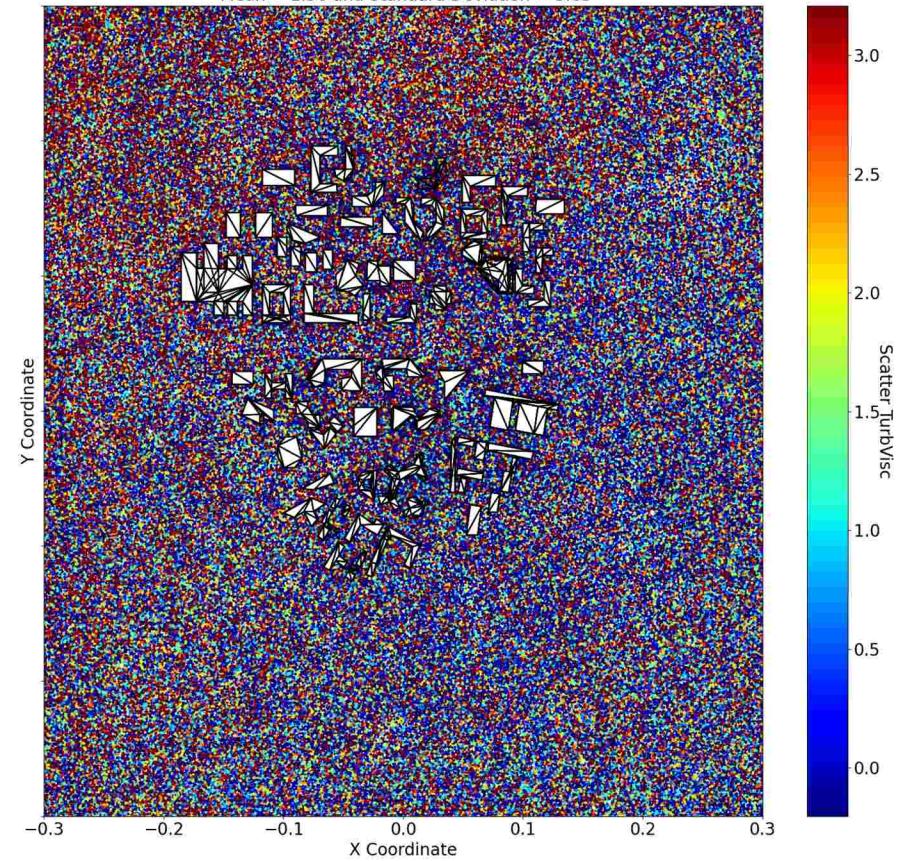
TurbVisc - Predicted

Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

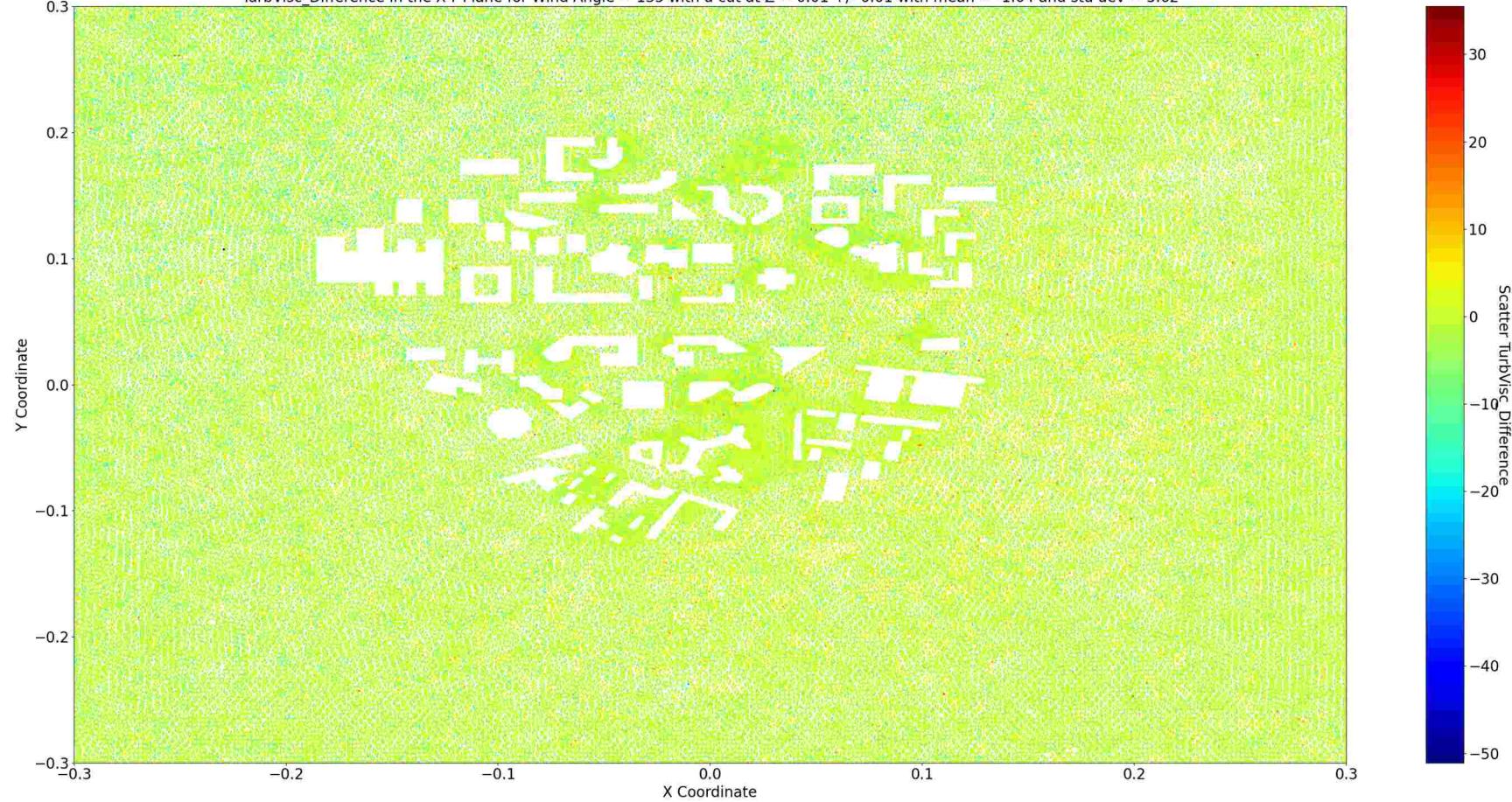
Actual TurbVisc in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.51 and Standard Deviation = 0.34



Predicted TurbVisc in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.56 and Standard Deviation = 3.63



TurbVisc_Difference in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01 with mean = -1.04 and std dev = 3.62



Proper Orthogonal Decomposition

Proper Orthogonal Decomposition

What went wrong?

- 1) No proper delineation between features (inputs to NN) and targets (outputs of NN) – not only are features and targets put together (which is probably not a good practice in general).
 - 1.1) Prediction angles that aren't 135 cannot be predicted in this manner as we only have the feature data and no target data to speak of – what we want IS the target data
 - 1.2) (I suppose we could put in a bunch of zeros as a form of dummy target data and ignore the MSE results since we only want the NN predictions but this seems a little problematic to say the least)

Proper Orthogonal Decomposition

What went wrong?

- 2) Correlating the columns even just for the targets alone means that we are saying that there is a linear relationship to be exploited in some finite N dimensions. I have no proof of this at all. I can only sketch a proof of linear correlations between the velocity components at best.
- 2.1) Even just by looking at RANS, it seems pretty obvious that it would be incredibly hard to approximate it linearly (or to find linear correlations between pressure, vx, vy, vz and nu_t).
- 3) Linearly correlating the rows I think is more or less ok to do. Eg at angle = 15, the values of vx should be linearly correlated with itself in some finite N dimensions. Similarly for vy, vz, pressure etc. And similarly for the rest of the angles. This proof can be sketched somewhat.

Proper Orthogonal Decomposition

How to fix?

- 1) Separate the features and targets into two distinct matrices. You must have a different set of eigenvectors for each.
- 2) Is doing POD row-wise enough? We do not correlate the target variables and/or angles when doing the full dataset either. The NN is supposed to learn the correlation for you.
- 3) Correlation between angles/variables is useful but perhaps a better way to do it is via non-linear methods (see autoencoders, kernel PCA, etc etc). The workload of the NN is reduced precisely because one tells it exactly what the correlations are.

Proper Orthogonal Decomposition

How to fix?

- 4) For the full dataset, the matrix size for the features is $(10^7, 60) \sim 6*10^8$ and the matrix size for the columns is $(10^7, 60)$ as well. The total size is $2*(6*10^8) = \sim 10^9$.
- 4.1) Compare to cylinder cell with $(10^5, 60) \sim 6*10^6$ for both features and targets. The total size is $\sim 10^7$.
- 4.2) Even if there was a non-linear correlation column wise that reduced the dimensions of the columns by 10 (doubtful) in both the features and targets, we could theoretically achieve one-tenth of cylinder-cell speeds for La Defense (~ 0.02 hours/epoch $\rightarrow 0.2$ hours/epoch) – (30,000 epochs takes ~ 250 days) [still way too long]

Proper Orthogonal Decomposition

How to fix?

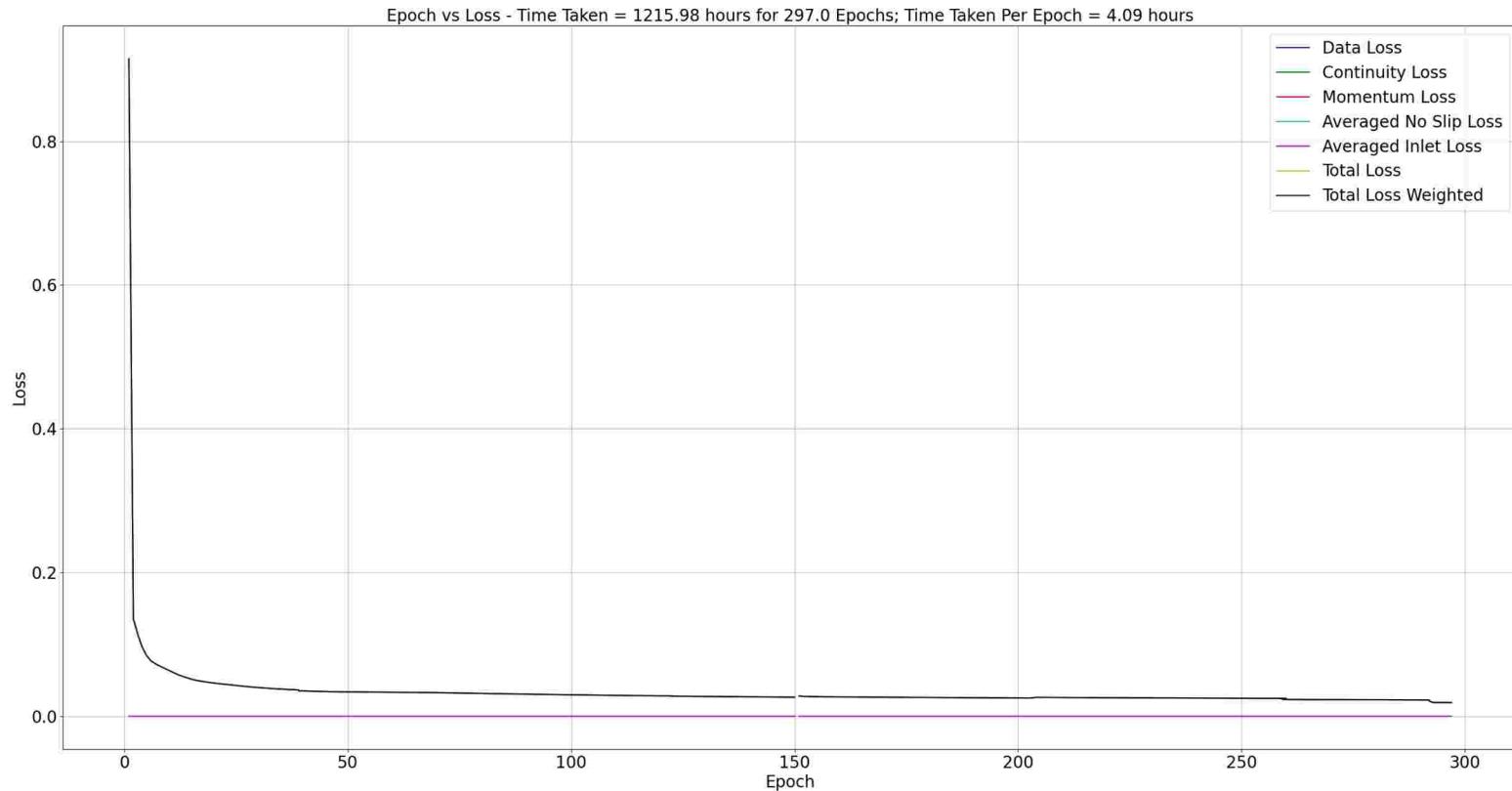
- 5) As a last approach, one could take pre-trained POD results and continue with full dataset training
 - 5.1) IE. output the NN predictions for POD at some N epochs, then read them in along with the CFD data on the normal NN architecture and train

Progress so far - Data Loss Only
Standard Normal Scalar – ELU Activation
(Adam Optimizer)

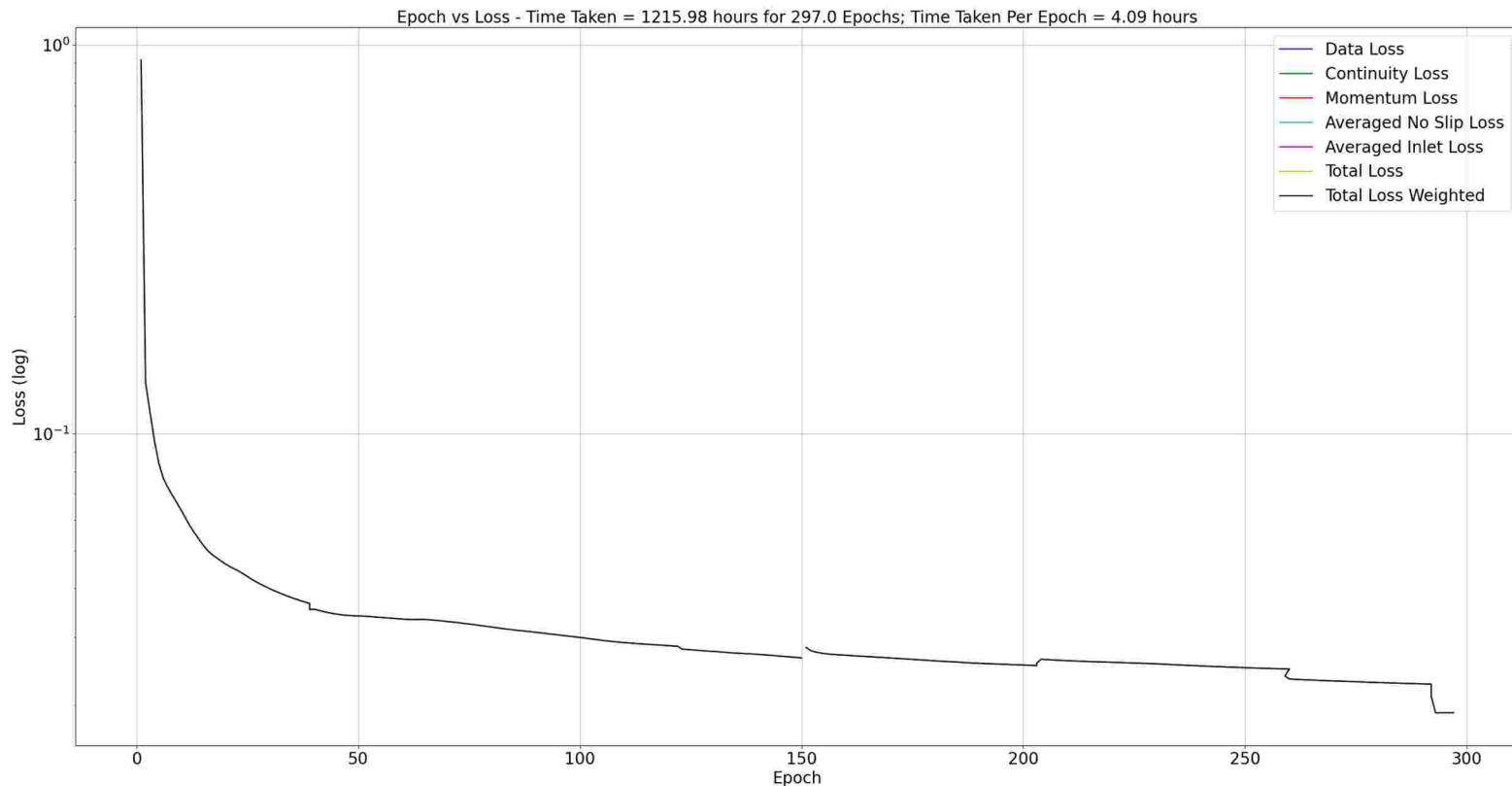
Full Dataset, GPU Workstation
297 Epochs

Scripts v5 – VALIDATION (135)

Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
297 Epochs, GPU Workstation
Data Loss Plot

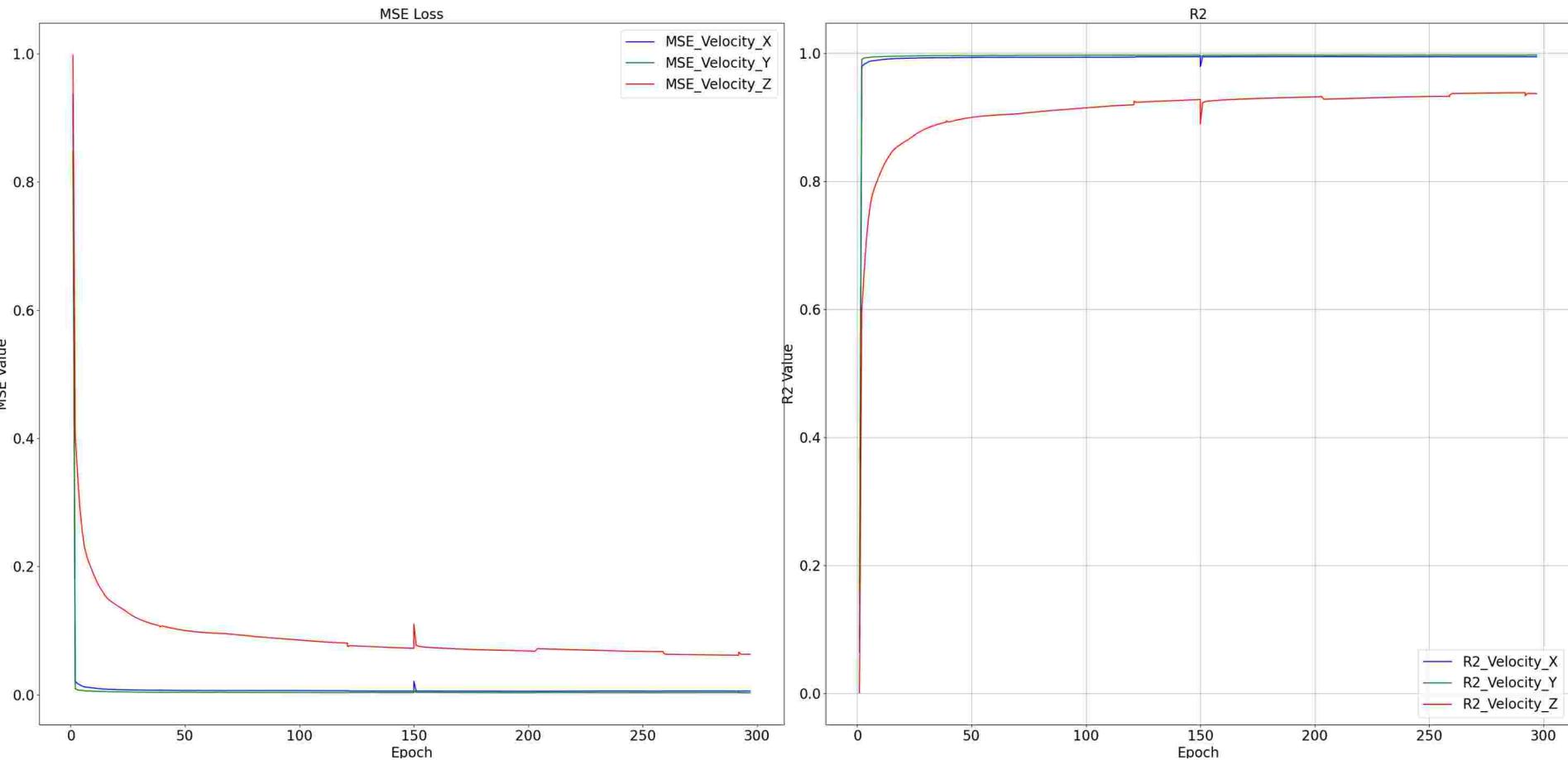


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
297 Epochs, GPU Workstation
Data Loss Plot



Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
297 Epochs, GPU Workstation
Training MSE & R2 Results

Time Taken = 1215.98 hours for 297.0 Epochs; Time Taken Per Epoch = 4.09 hours

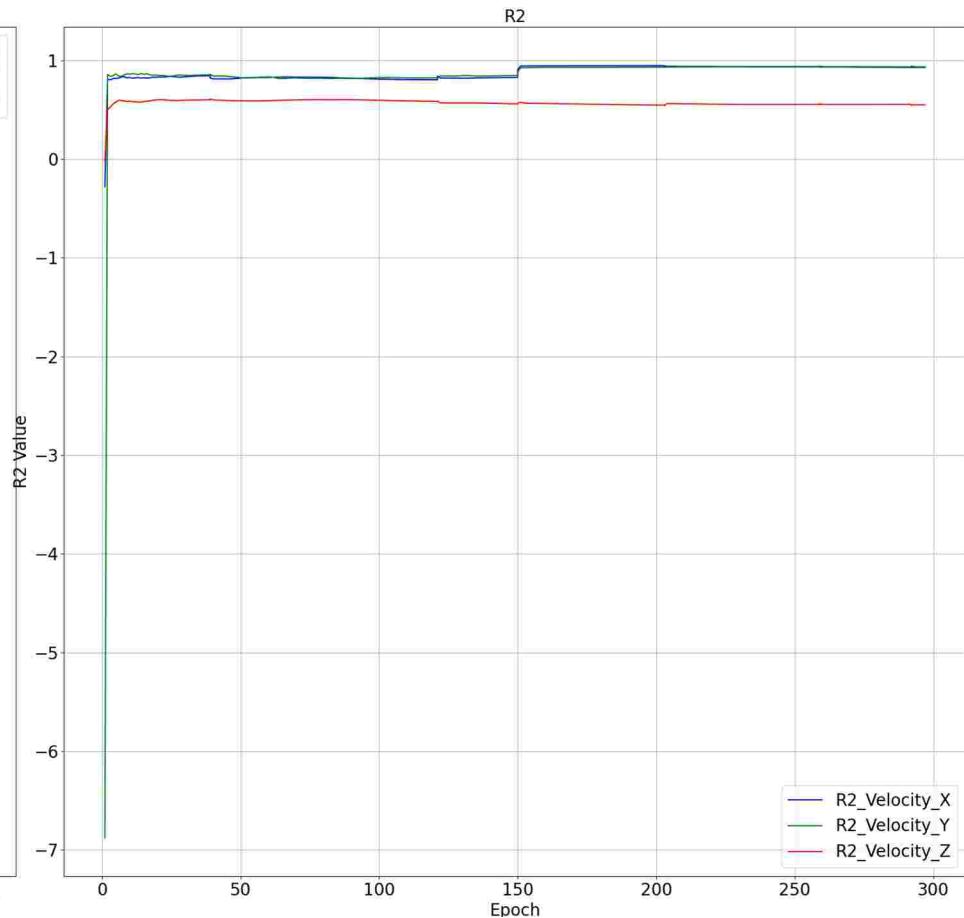
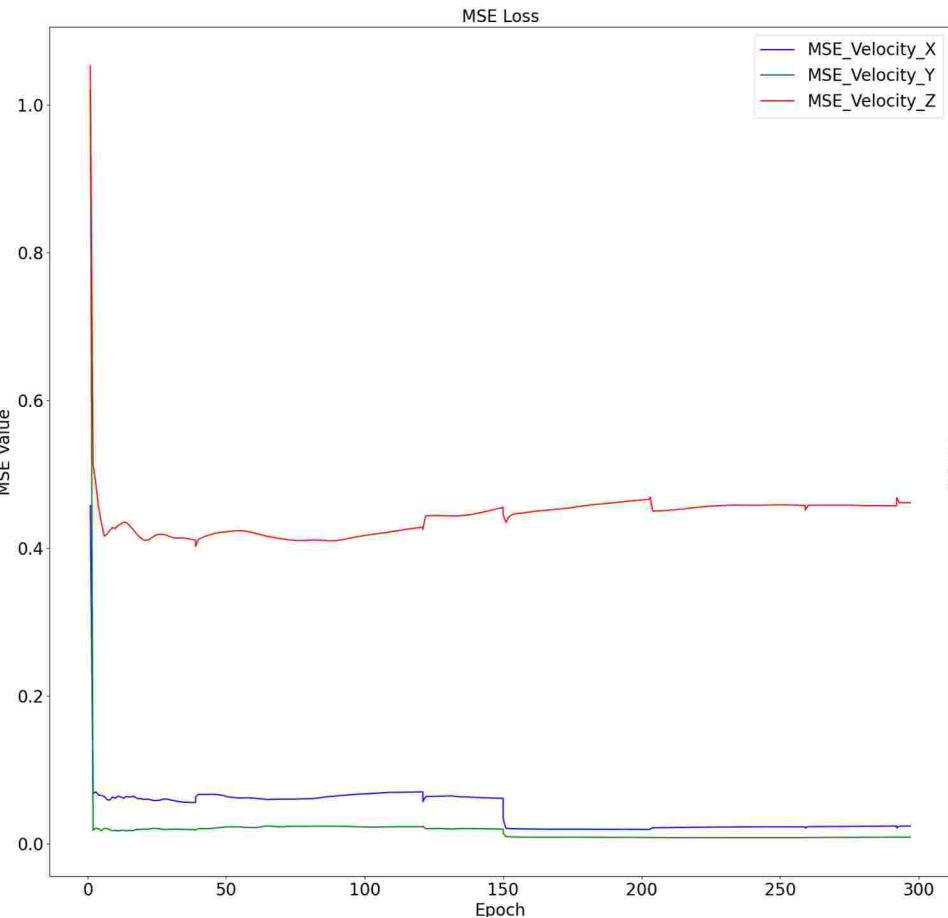


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer

297 Epochs, GPU Workstation

Validation MSE & R2 Results

Time Taken = 1215.98 hours for 297.0 Epochs; Time Taken Per Epoch = 4.09 hours

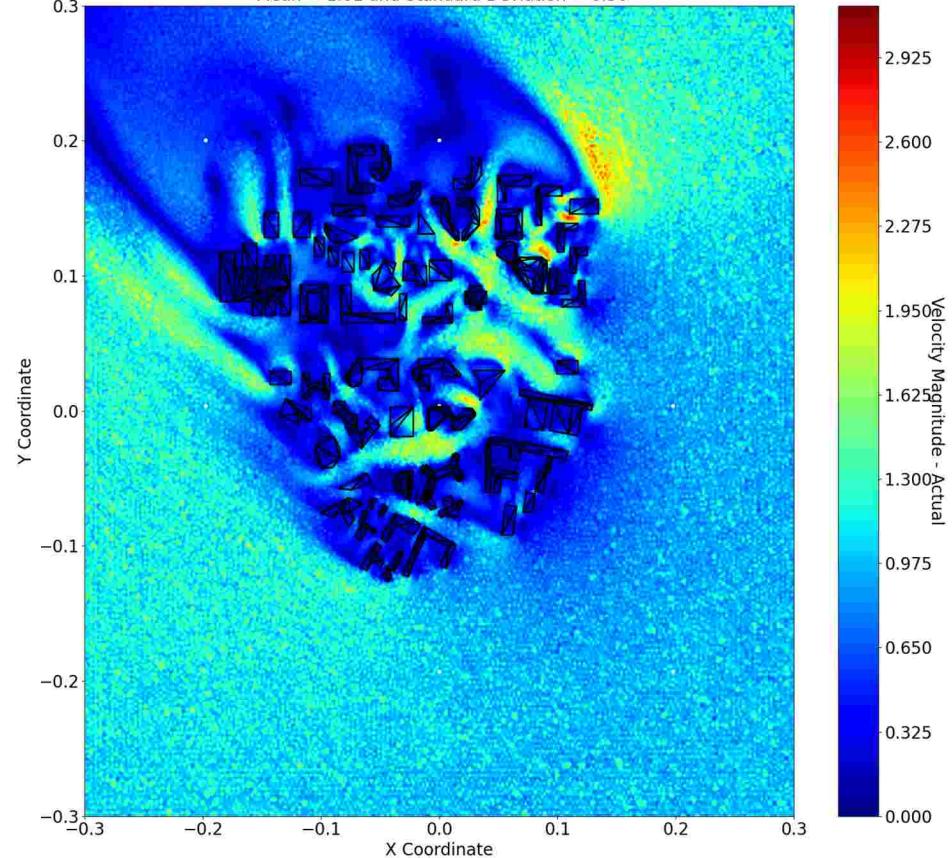


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
297 Epochs, GPU Workstation
Validation MSE & R2 Results

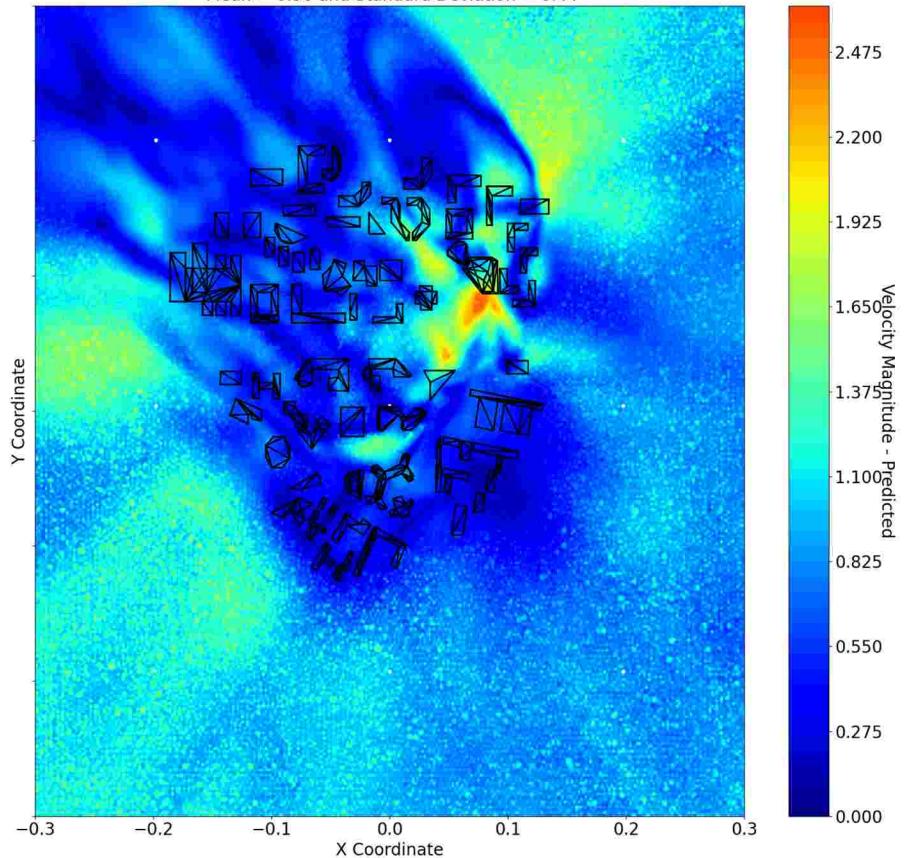
Variable	MSE	RMSE	MAE	R2
Velocity:0	0.071011418854	0.266479678126	0.178796765548	0.934199975550
Velocity:1	0.081488461361	0.285461838712	0.193012657734	0.928520592996
Velocity:2	0.008550792268	0.092470494044	0.035373776245	0.551391705232

Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.01 and Standard Deviation = 0.50

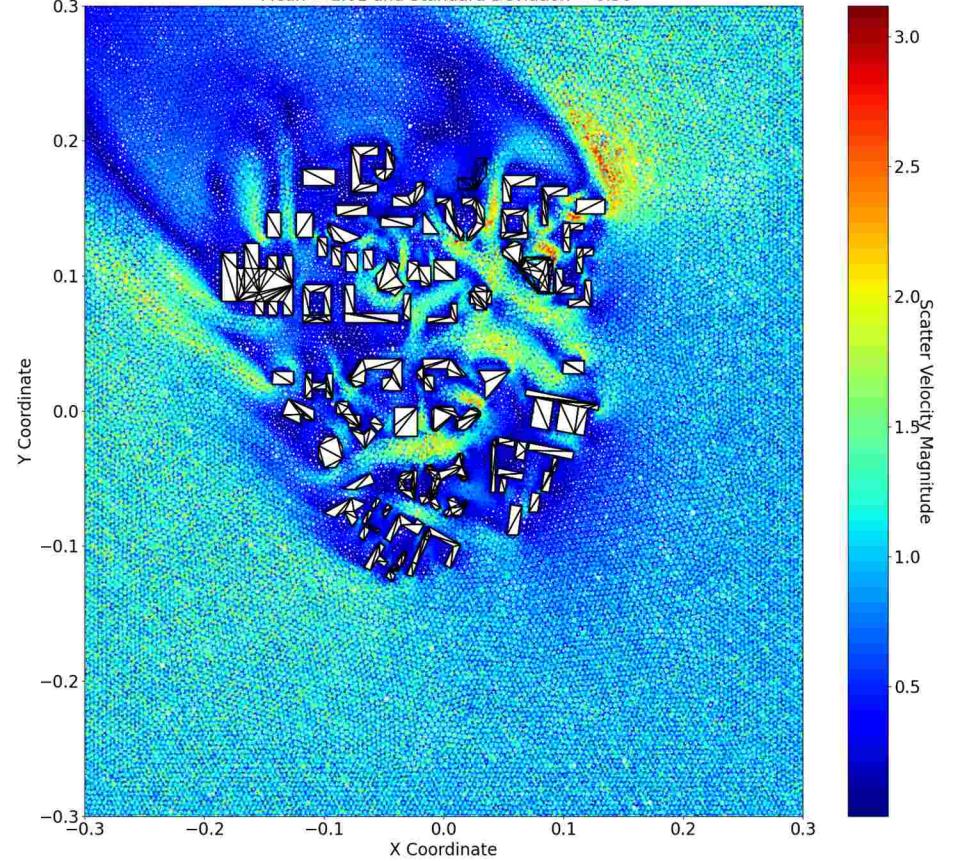


Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.96 and Standard Deviation = 0.44

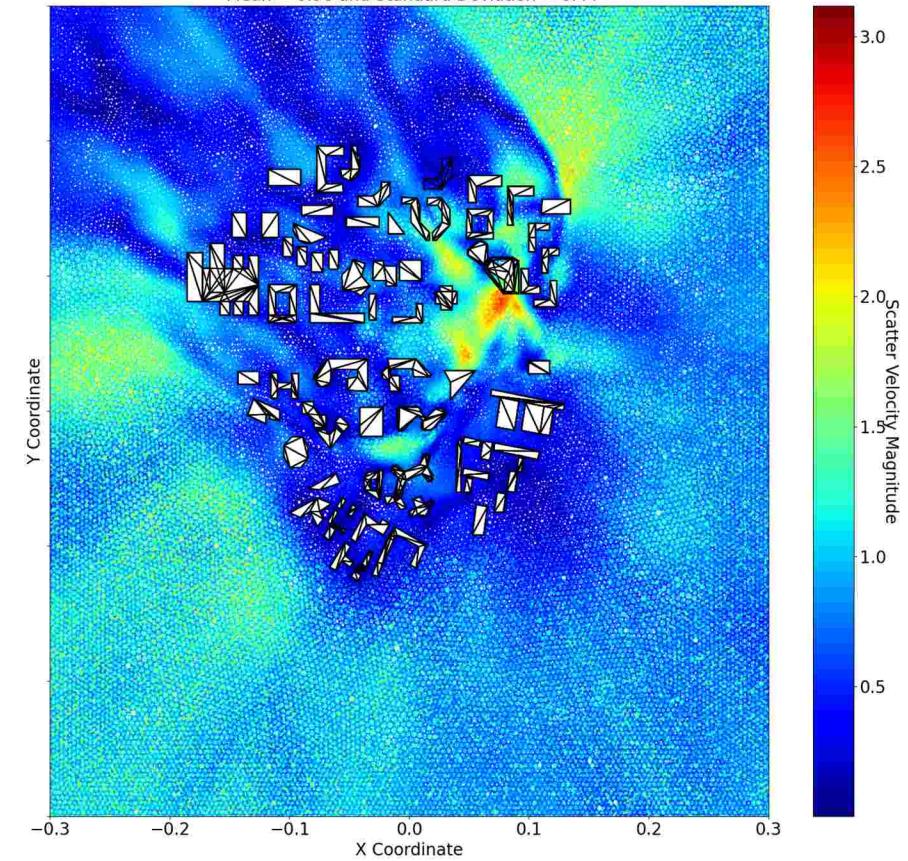


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

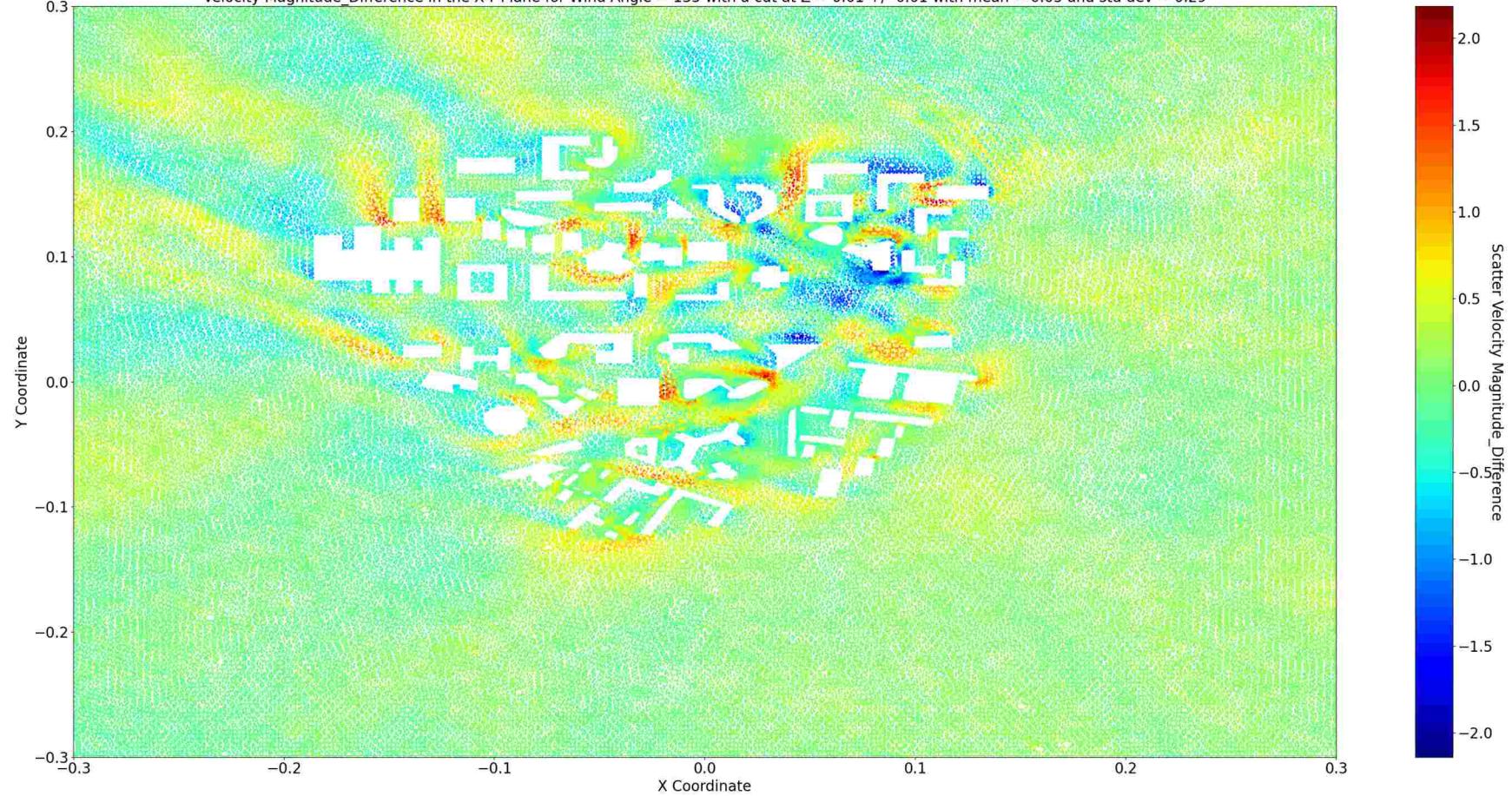
Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.01 and Standard Deviation = 0.50



Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 0.96 and Standard Deviation = 0.44



Velocity Magnitude_Difference in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01 with mean = 0.05 and std dev = 0.29

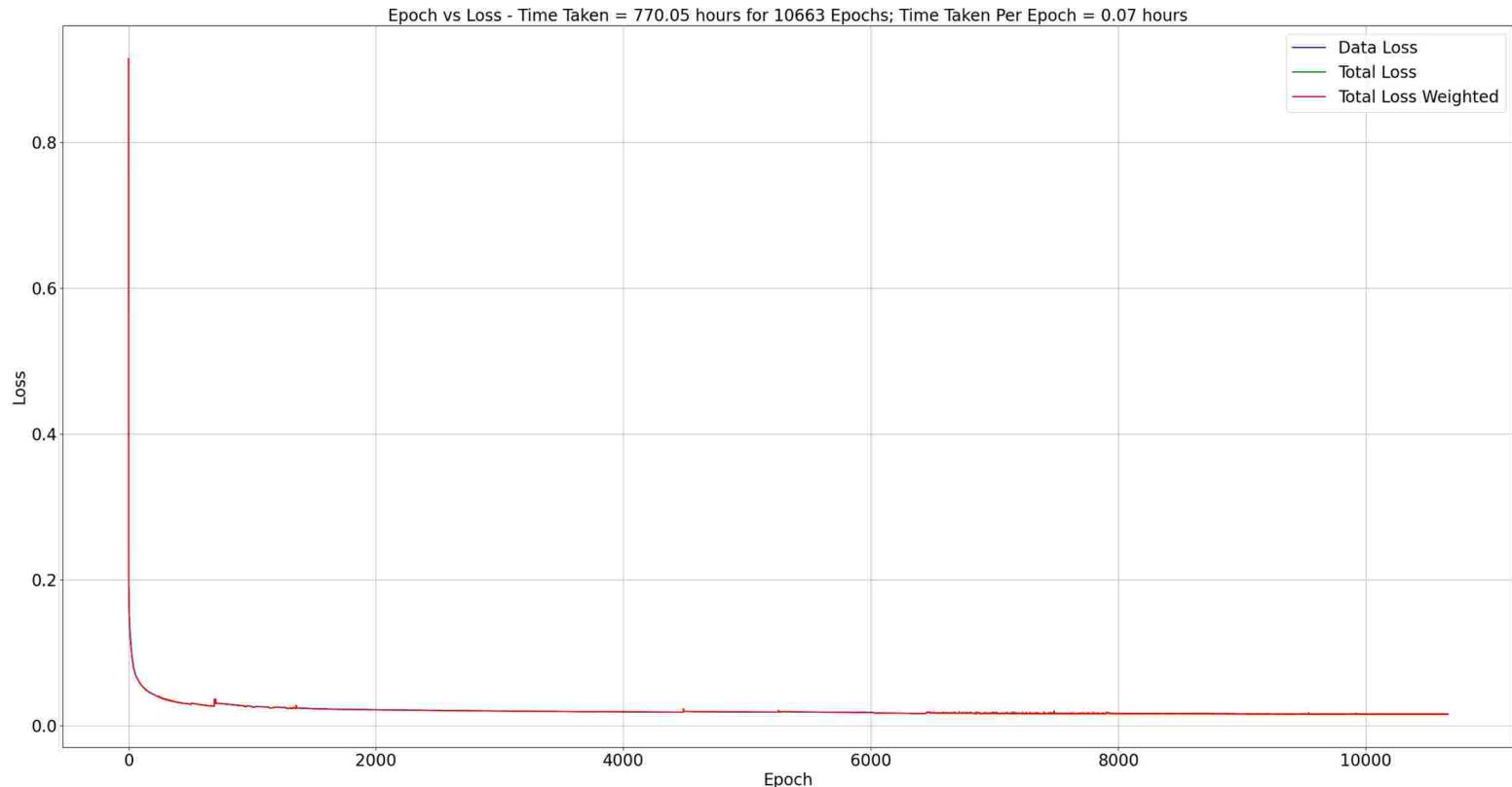


Progress so far - Data Loss Only
Standard Normal Scalar – ELU Activation
(Adam Optimizer)

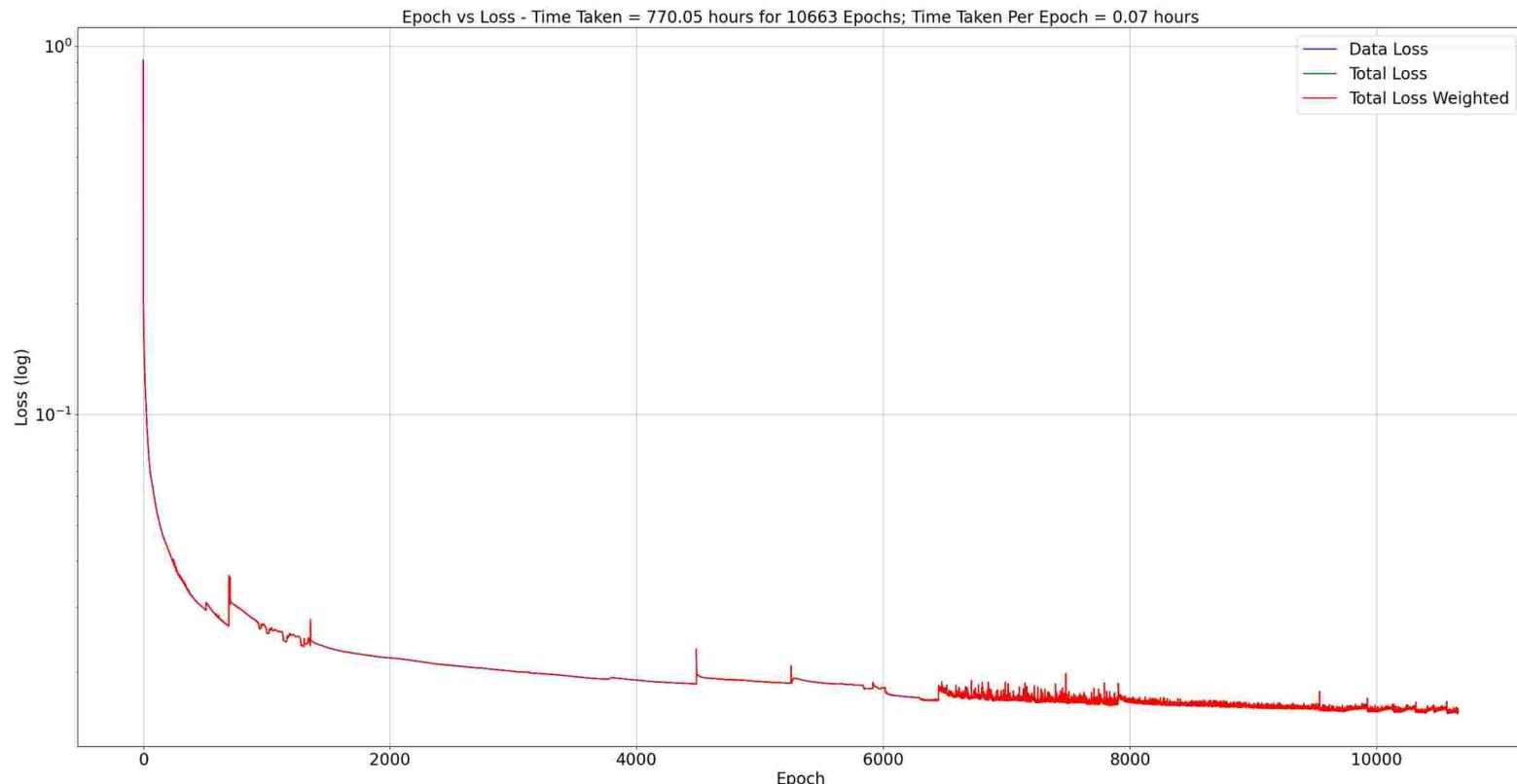
Sampled Dataset, GPU Laptop
10663 Epochs

Scripts v5 – VALIDATION (135)

Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
10663 Epochs, GPU Laptop
Data Loss Plot

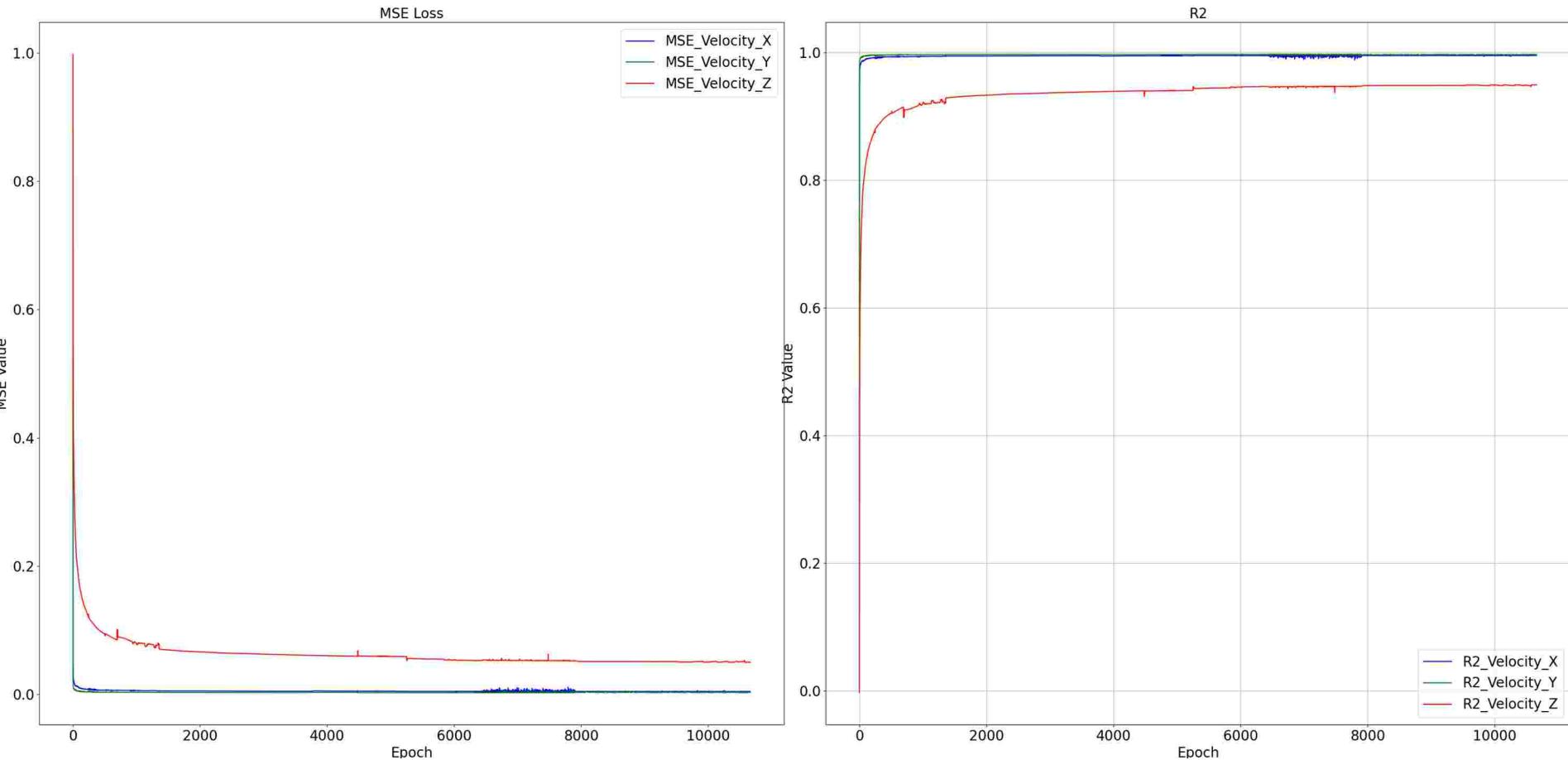


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
10663 Epochs, GPU Laptop
Data Loss Plot



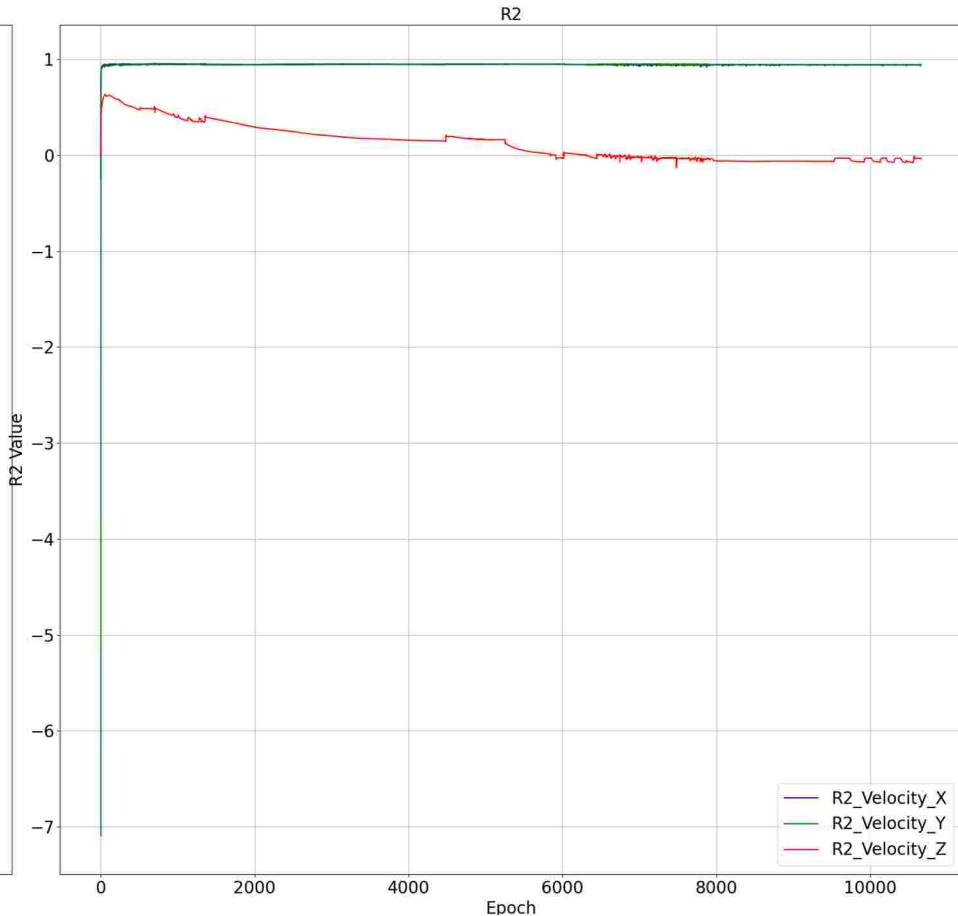
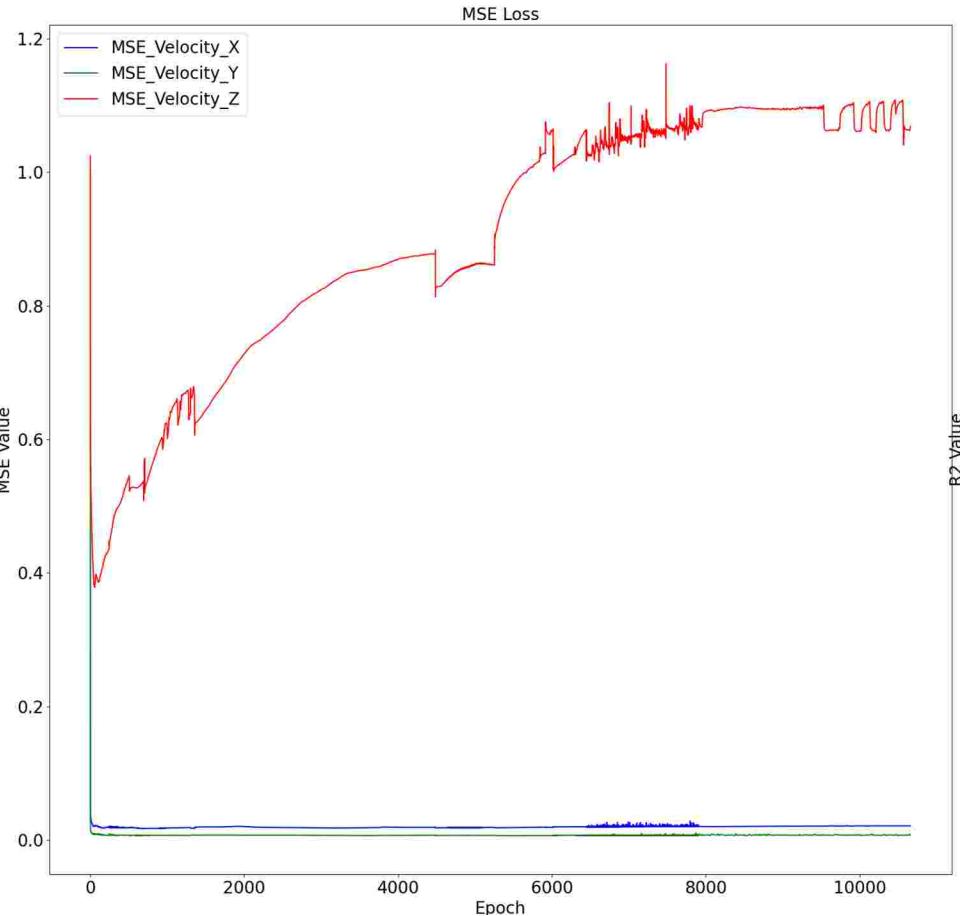
Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
10663 Epochs, GPU Laptop
Training MSE & R2 Results

Time Taken = 770.05 hours for 10663 Epochs; Time Taken Per Epoch = 0.07 hours



Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
10663 Epochs, GPU Laptop
Validation MSE & R2 Results

Time Taken = 770.05 hours for 10663 Epochs; Time Taken Per Epoch = 0.07 hours

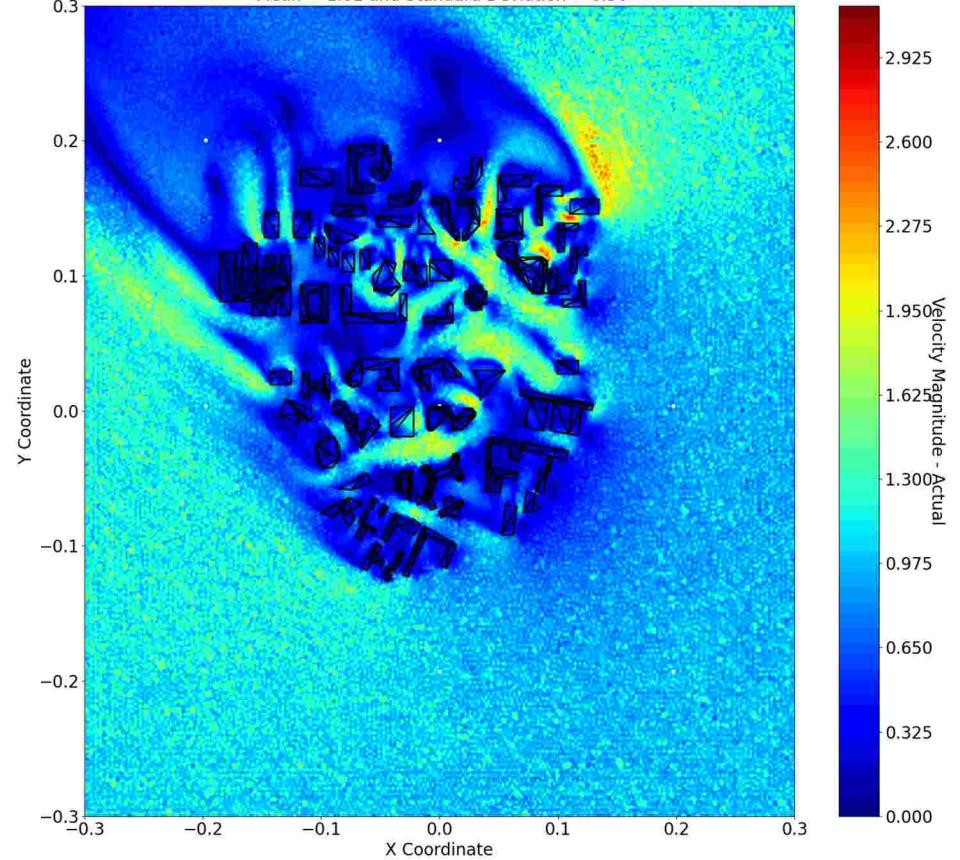


Progress so far - Data Loss Only, Standard Normal Scalar, ELU Activation, Adam Optimizer
10663 Epochs, GPU Laptop
Validation MSE & R2 Results

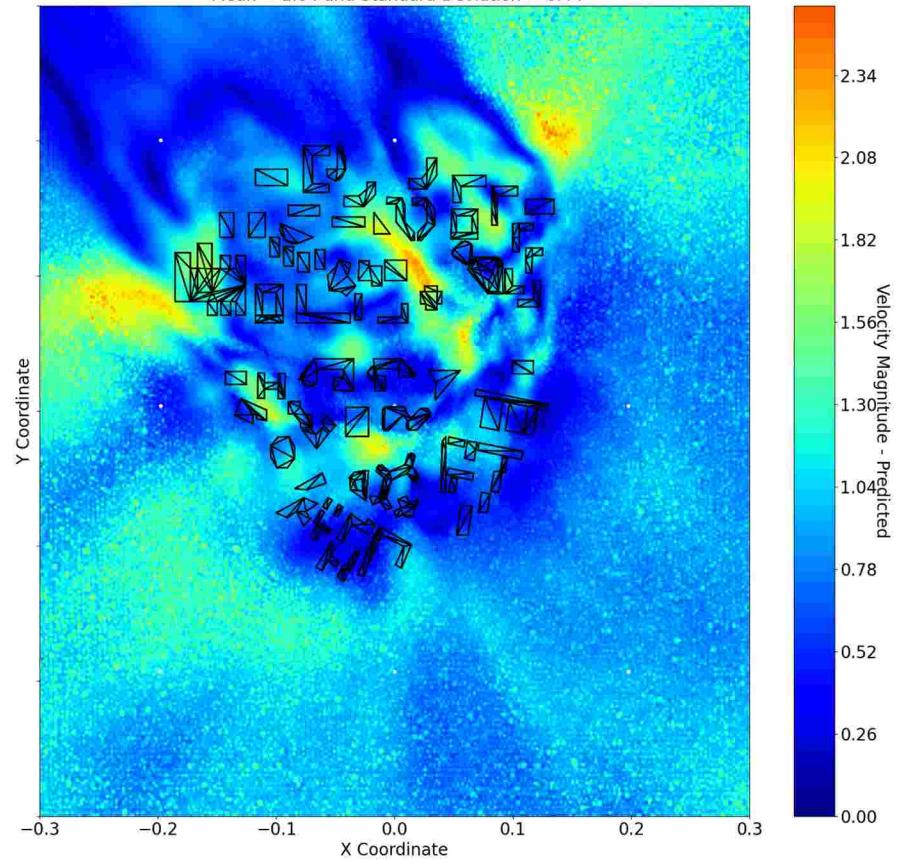
Variable	MSE	RMSE	MAE	R2
Velocity:0	0.062142287573	0.249283548541	0.129877784398	0.942418217976
Velocity:1	0.062632062665	0.250263985953	0.135808285918	0.945060900353
Velocity:2	0.019673133394	0.140260947504	0.045439598142	-0.032130187179

Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.01 and Standard Deviation = 0.50

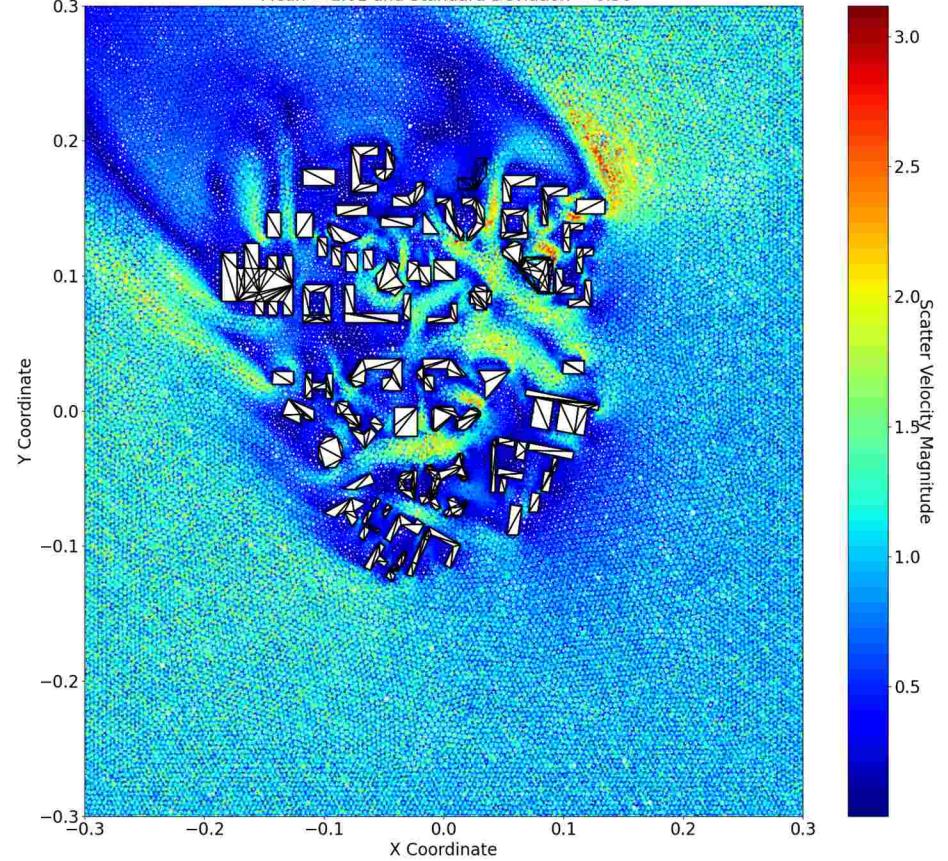


Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.04 and Standard Deviation = 0.44

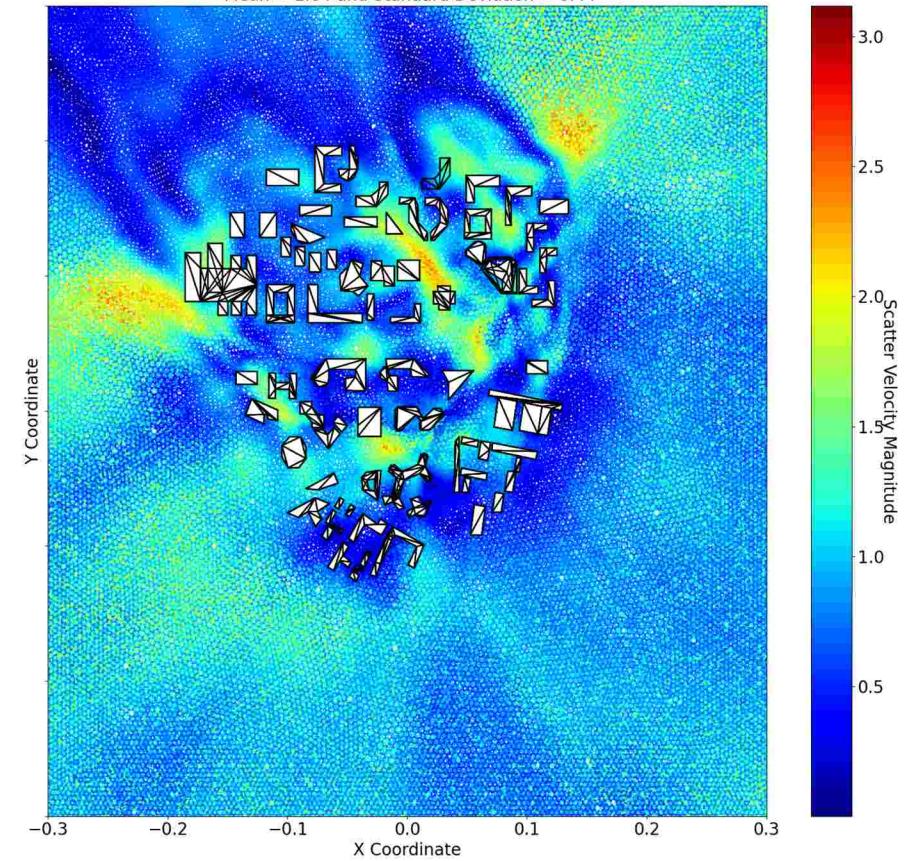


Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.01 +/- 0.01

Actual Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.01 and Standard Deviation = 0.50



Predicted Velocity Magnitude in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01
Mean = 1.04 and Standard Deviation = 0.44



Velocity Magnitude_Difference in the X-Y Plane for Wind Angle = 135 with a cut at Z = 0.01 +/- 0.01 with mean = -0.03 and std dev = 0.31

